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Micromechanical concept for the analysis of damage evolution in thermo-viscoelastic and quasi-brittle materials

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Abstract

The aim of this paper is to develop a thermodynamically consistent micromechanical concept for the damage analysis of viscoelastic and quasi-brittle materials. As kinematical damage variables a set of scalar-, vector-, and tensor-valued functions is chosen to describe isotropic and anisotropic damage. Since the process of material degradation is governed by physical mechanisms on levels with different length scale, the macro- and mesolevel, where on the mesolevel microdefects evolve due to microforces, we formulate in this paper the dynamical balance laws for macro- and microforces and the first and second law of thermodynamics for macro- and mesolevel.

Assuming a general form of the constitutive equations for thermo-viscoelastic and quasi-brittle materials, it is shown that according to the restrictions imposed by the Clausius–Duhem inequality macro- and microforces consist of two parts, a non-dissipative and a dissipative part, where on the mesolevel the latter can be regarded as driving forces on moving microdefects. It is shown that the non-dissipative forces can be derived from a free energy potential and the dissipative forces from a dissipation pseudo-potential, if its existence can be assured.

The micromechanical damage theory presented in this paper can be considered as a framework which enables the formulation of various weakly nonlocal and gradient, respectively, damage models. This is outlined in detail for isotropic and anisotropic damage.

Keywords: Microstructure; Nonlocal damage; Gradient damage theory; Anisotropic damage; Brittle damage; Evolution laws

1. Introduction

Local damage models for brittle and ductile materials were extensively discussed in the literature (e.g. Kachanov, 1958, 1986; Ortiz, 1985; Simo and Ju, 1987; Chaboche, 1988; Lemaitre, 1992; Krajcinovic, 1996). In local phenomenological theories, the damage parameters are considered as internal variables, for which evolution laws have to be given. Besides the fact that it is difficult to determine appropriate damage evolution laws, the FE-solutions based on local damage theories suffer from strong mesh-dependency, if problems with damage localization are analyzed. Also it was observed that the so-called size effect of

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structures cannot be simulated by local damage models (cf. Bažant and Ožbolt, 1990; Bažant and Planas, 1998). The reason for these difficulties lies in the fact that material degradation during the lifetime of structures is governed by physical mechanisms on levels with different length scale, the macro- and meso- or microlevel. In brittle material microcracks and microvoids and in ductile material microvoids, microshearbands and dislocations are observed, which can evolve relative to the surrounding material.

To overcome the numerical difficulties associated with the application of FE-solution methods, based on local damage theories, integral enhancement (e.g. Bažant and Pijaudier-Cabot, 1988; Bažant, 1991) and gradient enhancement (e.g. de Borst et al., 1996; Kuhl et al., 2000; Geers et al., 2000) were introduced into local damage models. Also, applying local models of finite elastoplasticity, strong mesh-dependency of the FE-solutions is observed, if localization of the plastic deformation occurs (e.g. Roehl and Ramm, 1996; Miehe, 1998; Schieck et al., 1999). Here also, gradient-enhanced models of plasticity were proposed (e.g. de Borst and Mühlhaus, 1992). These models can be considered as phenomenological theories with weakly nonlocal enhancement: damage and plasticity variables are treated as internal variables, for which evolution laws have to be assumed, and strain or hardening parameters are enhanced by second gradient terms.

To model the material behavior on levels with different length scale a quite different approach is applied e.g. in Capriz, 1989; Marshall et al., 1991; Naghdi and Srinivasa, 1993; Fried and Gurtin, 1994; Le and Stumpf, 1996 and Frémond and Nedjar, 1996. In these papers theories are investigated, where besides the balance laws of macroforces also balance laws of microforces are formulated. To model the material behavior on levels with different length scale taking into account discontinuous fields of defects a six-dimensional kinematical concept with non-Euclidean space structure is introduced in Stumpf and Saczuk, 2000 and Saczuk et al., 2001. There, balance laws of macroforces and microforces are derived applying a variational formulation. Rakotomanana (2002) presents a kinematical theory of continua with discontinuous fields of defects on the mesolevel. As application he investigates the measuring of the loss in an ultrasonic signal due to propagation through defected in situ structures.

Thermodynamically consistent frameworks for a damage analysis published in the literature so far are mainly devoted to phenomenological theories, where the fields of plasticity and damage are treated as internal variables, for which evolution laws have to be postulated (e.g. Hansen and Schreyer, 1994; Arnold and Saleeb, 1994; Li, 1999). In Svedberg and Runesson (1997) the internal variable approach is investigated for isothermal plasticity with coupling to isotropic damage, where for regularization reason a gradient-enhancement of the isotropic hardening parameter is introduced.

The aim of this paper is to present a thermodynamically consistent micromechanical concept for the analysis of isotropic and anisotropic damage evolution in thermo-viscoelastic and quasi-brittle materials. Since our goal is the modeling of consistent damage theories simple enough to construct appropriate FE solution algorithms and to analyze the degradation of engineering structures, we use an Euclidean space concept with classical gradient operator. To take into account anisotropic damage a damage variable of scalar-, vector- and tensor-type or any combination thereof is introduced (see also Krajcinovic, 1998). Since the degradation of material is essentially caused by nucleation and evolution of microdefects as microcracks, microvoids and dislocations on a mesolevel, and this evolution of the microdefects is caused by microforces, we formulate dynamical balance laws for macro- and microforces and the first and second law of thermodynamics for the macro- and mesolevel. Microdefects move relative to the surrounding mass. Therefore, in the dynamical balance laws for microforces we take into account the rate of micromomentum and in the balance law of energy the kinetic energy of moving microdefects, both independent of the mass.

For thermo-viscoelastic material behavior, we assume the constitutive equations for macro- and microforces and heat transfer in general form. It is then shown that from the restrictions imposed by the Clausius–Duhem inequality, macro- as well as microforces consist of two parts, a non-dissipative and a dissipative part. On the mesolevel the latter represent the driving forces on microdefects causing their dissipative evolution. Corresponding to the split of macro- and microforces into non-dissipative and dissipative parts, the constitutive equations can be represented via a free energy potential and a dissipation pseudo-potential, if the latter exists. Then, from the free energy potential the non-dissipative forces and from the dissipative pseudo-potential the dissipative driving forces follow.

Considering the presented micromechanical damage theory as a framework, various weakly nonlocal and gradient, respectively, isotropic and anisotropic damage models can be derived. For numerical applications of special importance are anisotropic damage models, where the gradients of some damage variables can be neglected. In this case, the corresponding balance laws of microforces lead directly to evolution laws for these damage variables.

The organization of the paper is as follows.

In Section 2, the micromechanical modeling of damage phenomena is investigated by formulating dynamical balance laws of macro- and microforces and the first and second law of thermodynamics for macro- and mesolevel. Constitutive equations for thermo-viscoelastic and quasi-brittle materials coupled with damage are assumed in general form, where the constitutive restrictions follow from the Clausius–Duhem inequality. It is shown that macro- and microforces consist of two parts, a non-dissipative and a dissipative part. Introducing the constitutive equations into the balance laws of macro- and microforces leads to the governing equations of dynamical defect evolution.

In Section 3, the isotropic damage described by a scalar function is investigated for various classes of material properties and process data. In Section 4, we consider the case of anisotropic damage. If the anisotropy is described by an anisotropy tensor, then the procedure of specification and simplification outlined for isotropic damage in Section 3 can be applied correspondingly. In the case of an anisotropic damage description with a scalar and an anisotropy tensor, it is often possible to assume that the gradient of the anisotropy tensor can be neglected, while the gradient of the scalar function has to be taken into account. It is shown that in this case the evolution law for the anisotropy tensor can be derived directly from the corresponding balance law of microforces.

2. Micromechanical modeling of damage phenomena

The following notation scheme is used. The three-dimensional Euclidean point space is denoted by $\mathscr{E}$ and the associated translation space (the three-dimensional Euclidean vector space) by E. Moreover, vectors are denoted by lower case bold letters and multilinear operators (tensors) by upper case bold letters. Whenever finite dimensional vector spaces are considered we shall identify the tensor product vector space $F \otimes E$ with the vector space $L(E, F)$ of all linear maps of the vector space E into any other inner product vector space F. We write $\boldsymbol{u} \cdot \boldsymbol{w}$ for the inner product of vectors regardless of the vector space in question. We also recall that the inner product of two tensors (linear maps) $\boldsymbol{A}, \boldsymbol{B} \in L(E, F)$ is defined by $\boldsymbol{A} \cdot \boldsymbol{B} = \mathrm{tr}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{B})$, where $\boldsymbol{A}^{\mathrm{T}}, \boldsymbol{B}^{\mathrm{T}} \in L(F, E)$ and "tr" denotes the trace of the tensor.

2.1. Damage variables and kinematics of damaged bodies

For the purpose of this paper, the material body under consideration may be identified with a region $B_0 \subset \mathscr{E}$ in the physical space, which the body occupies in a fixed reference configuration. The motion of the body is then described by a mapping $\boldsymbol{\chi} : B_0 \times T \to \mathscr{E}$, which carries each material particle $\mathbf{X} \in B_0$ into its place $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t)$ in the spatial configuration $B(t) = \boldsymbol{\chi}(B_0, t)$ of the body at time instant t, where T denotes the underlying time interval. Once the mapping $\boldsymbol{\chi}$ is specified, all kinematic variables on the macrolevel such as velocity, deformation gradient, strain tensors, etc., are defined in the standard manner (Truesdell and Noll, 1965).

To account for the physical mechanisms underlying the damage process on macro- and mesolevel, a reformulation of the kinematical concept and of some principles of classical continuum thermomechanics is required. On the macroscale, the damage process is described by introducing certain damage variables, which can be viewed as macroscopic measures of the internal degradation of the material. In this paper, we shall assume that the state of damage in a material can be characterized by a damage variable $\mathbf{d}(\boldsymbol{X},t)$ of any nature (scalar, vector or tensor). We also admit that $\mathbf{d}$ may represent an ordered collection of any number of damage variables possibly of different nature, e.g. $\mathbf{d} \equiv (d, \boldsymbol{d}, \boldsymbol{D})$ consisting of a scalar d, a vector $\boldsymbol{d}$, and a second rank tensor $\boldsymbol{D}$. For definiteness and proper mathematical setting, we assume that $\boldsymbol{d} : B_0 \times T \to F$, where F is a finite-dimensional inner product vector space (e.g. $\mathbb{R}$, $\otimes^p E$ or $\oplus^p E$ for some $p \geqslant 1$, $\mathbb{R} \oplus E \oplus (E \otimes E)$, etc.) and we shall refer to F as a "damage space".

2.2. Integral laws of mechanics and thermodynamics on macro- and mesolevel

Experimentally observed progressive degradation of mechanical and thermal properties of continua is governed by physical mechanisms observed on levels with different length scale, on macro-, meso-, and microlevel, respectively. In brittle material there can be microdefects as microcracks and microvoids, in ductile material microvoids, dislocations and microshearbands. While the precise physical nature of the microdefects can be difficult to identify for a specific material, it is obvious that the nucleation and evolution of the microdefects are caused by forces on the mesolevel. This suggests to postulate additional balance laws for microforces, besides the classical balance laws of forces on the macrolevel. Within such two-level modeling of damage phenomena the first and second law of thermodynamics have to be modified taking into account the contributions from the mesolevel.

We assume that the referential mass density $\varrho_0(\boldsymbol{X})$ is independent of time. The balance laws of macromomentum and angular macromomentum can be given as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\int_{P_0} \boldsymbol{p}\,\mathrm{d}v &= \int_{P_0} \boldsymbol{b}\,\mathrm{d}v + \int_{\partial P_0} \boldsymbol{T}\boldsymbol{n}_0\,\mathrm{d}a, \\ \frac{\mathrm{d}}{\mathrm{d}t}\int_{P_0} \boldsymbol{x}\times\boldsymbol{p}\,\mathrm{d}v &= \int_{P_0} \boldsymbol{x}\times\boldsymbol{b}\,\mathrm{d}v + \int_{\partial P_0} \boldsymbol{x}\times\boldsymbol{T}\boldsymbol{n}_0\,\mathrm{d}a. \end{aligned} \tag{2.1}$$

Here $\boldsymbol{p}(\boldsymbol{X},t) \in E$ denotes the macromomentum, $\boldsymbol{b}(\boldsymbol{X},t) \in E$ the classical body force, $\boldsymbol{T}(\boldsymbol{X},t) \in E \otimes E$ the first Piola–Kirchhoff stress tensor, $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X},t)$ the place of a material point in the actual configuration, and $\boldsymbol{n}_0(\boldsymbol{X})$ the outward unit normal vector to the boundary ∂P_0 of a subdomain $P_0 \subset B_0$.

To formulate the balance law of microforces, we assume that the microdefects are characterized by a "damage" field $\mathbf{d} : B_0 \times T \to F$ and that at each time instant the stress state on the mesolevel may be characterized by an intrinsic microforce $\mathbf{k}(\boldsymbol{X},t) \in F$, an extrinsic microforce $\mathbf{g}(\boldsymbol{X},t) \in F$ representing e.g. chemical reactions breaking internal material bonds, and a microstress tensor $\mathbf{H}(\boldsymbol{X},t) \in F \otimes E$. Then, the balance of microforces can be given as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{P_0} \mathbf{m}\,\mathrm{d}v = \int_{P_0} (-\mathbf{k}+\mathbf{g})\,\mathrm{d}v + \int_{\partial P_0} \mathbf{H}\boldsymbol{n}_0\,\mathrm{d}a. \tag{2.2}$$

Evolving microdefects have no mass but they have inertia. This effect is included in the present theory through the micromomentum $\mathbf{m}(\boldsymbol{X},t)$. We have to point out that the integration of the terms in (2.2) has to be performed over the same subdomain $P_0 \subset B_0$ and the boundary surface ∂P_0 as in (2.1).

Besides the balance laws for macro- and microforces we have to formulate the first law of thermodynamics on macro- and mesolevel taking into account also the kinetic energy of evolving defects, the contribution of the extrinsic microforce $\mathbf{g}$ in the interior of P_0 and of the surface microforce $\mathbf{H}\boldsymbol{n}_0$ on the surface ∂P_0

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_{P_0} (\varrho_0\varepsilon+\kappa)\,\mathrm{d}v\right\} = \int_{P_0} (\boldsymbol{b}\cdot\dot{\boldsymbol{x}}+\mathbf{g}\cdot\dot{\mathbf{d}}+\varrho_0 r)\,\mathrm{d}v + \int_{\partial P_0} (\boldsymbol{T}\boldsymbol{n}_0\cdot\dot{\boldsymbol{x}}+\mathbf{H}\boldsymbol{n}_0\cdot\dot{\mathbf{d}}-\boldsymbol{q}\cdot\boldsymbol{n}_0)\,\mathrm{d}a. \tag{2.3}$$

Here $\varepsilon(\boldsymbol{X}, t) \in \mathbb{R}$ denotes the specific internal energy, $\kappa(\boldsymbol{X}, t) \in \mathbb{R}$ the specific kinetic energy, $r(\boldsymbol{X}, t) \in \mathbb{R}$ the external body heating, and $\boldsymbol{q}(\boldsymbol{X}, t) \in E$ the referential heat flux vector.

The specific kinetic energy for macro- and mesolevel is assumed in the form

$$\kappa(\dot{\boldsymbol{x}}, \dot{\boldsymbol{d}}) = \frac{1}{2}\varrho_0 \dot{\boldsymbol{x}} \cdot \dot{\boldsymbol{x}} + \frac{1}{2}\varrho_0 \mathbf{A}\dot{\mathbf{d}} \cdot \dot{\mathbf{d}}, \tag{2.4}$$

where $\mathbf{A}$ is the microinertia tensor, which is independent of the mass. For simplicity, we assume that $\mathbf{A}$ is time-independent. Macromomentum $\boldsymbol{p}$ and micromomentum $\mathbf{m}$ are related to the kinetic energy κ as follows

$$\boldsymbol{p} = \frac{\partial \kappa}{\partial \dot{\boldsymbol{x}}_{|\dot{\boldsymbol{d}}}} = \varrho_0 \dot{\boldsymbol{x}}, \quad \mathbf{m} = \frac{\partial \kappa}{\partial \dot{\mathbf{d}}_{|\dot{\boldsymbol{x}}}} = \varrho_0 \mathbf{A}\dot{\mathbf{d}}. \tag{2.5}$$

The balance laws (2.1)–(2.3) must be supplemented by the Clausius–Duhem inequality

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{P_0} \varrho_0 \eta \, \mathrm{d}v \geqslant \int_{P_0} \theta^{-1} r \, \mathrm{d}v - \int_{\partial P_0} \theta^{-1} \boldsymbol{q} \cdot \boldsymbol{n}_0 \, \mathrm{d}a \tag{2.6}$$

regarded as an appropriate statement of the second law of thermodynamics. Here $\eta(\boldsymbol{X}, t) \in \mathbb{R}$ is the specific entropy and $\theta(\boldsymbol{X}, t) \in \mathbb{R}^+$ the absolute temperature.

2.3. Local laws of micro-thermodynamics

Analogous to the classical theories of continuum thermodynamics, the laws of mechanics and thermodynamics on macro- and mesolevel are assumed to hold for every $P \subset B$. Under the usual regularity requirements the classical local equations of macromotion follow from (2.1) (Marsden and Hughes, 1983, p. 135)

$$\mathrm{Div}\boldsymbol{T} + \boldsymbol{b} = \dot{\boldsymbol{p}}, \quad \boldsymbol{T}\boldsymbol{F}^{\mathrm{T}} - \boldsymbol{F}\boldsymbol{T}^{\mathrm{T}} = \boldsymbol{0} \tag{2.7}$$

and the local equations of micromotion follow from (2.2)

$$\mathrm{Div}\mathbf{H} - \mathbf{k} + \mathbf{g} = \dot{\mathbf{m}}, \tag{2.8}$$

where $\dot{\boldsymbol{p}}$ and $\dot{\mathbf{m}}$ represent the rates of macro- and micromomenta (2.5). In (2.7) and (2.8) and subsequently the gradient operator $\nabla \equiv \mathrm{Grad}$ and the divergence operator Div are defined with respect to the reference configuration B_0.

Under the assumption that Eqs. $(2.7)_1$ and (2.8) are satisfied, the global energy balance (2.3) leads to the rate of the internal energy

$$\varrho_0 \dot{\varepsilon} = \boldsymbol{T} \cdot \dot{\boldsymbol{F}} + \mathbf{k} \cdot \dot{\mathbf{d}} + \mathbf{H} \cdot \nabla \dot{\mathbf{d}} + \varrho_0 r - \mathrm{Div}\boldsymbol{q}. \tag{2.9}$$

The first term on the right-hand side of (2.9) may also be written as

$$\boldsymbol{T} \cdot \dot{\boldsymbol{F}} = \frac{1}{2}\boldsymbol{S} \cdot \dot{\boldsymbol{C}} = \boldsymbol{S} \cdot \dot{\boldsymbol{E}}, \tag{2.10}$$

where $\boldsymbol{S}(\boldsymbol{X}, t)$ denotes the second Piola–Kirchhoff stress tensor, $\boldsymbol{C}(\boldsymbol{X}, t)$ the right Cauchy–Green deformation tensor and $\boldsymbol{E}(\boldsymbol{X}, t)$ the Green strain tensor (all being $E \otimes E$-valued fields):

$$\boldsymbol{T} = \boldsymbol{F}\boldsymbol{S}, \quad \boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}, \quad \boldsymbol{E} = \frac{1}{2}(\boldsymbol{C} - \boldsymbol{1}). \tag{2.11}$$

With the assumption that the Clausius–Duhem inequality (2.6) is the appropriate form of the second law of thermodynamics, the local dissipation inequality for macro- and mesolevel is obtained as

$$\mathscr{D} \equiv \boldsymbol{T} \cdot \dot{\boldsymbol{F}} + \mathbf{k} \cdot \dot{\mathbf{d}} + \mathbf{H} \cdot \nabla \dot{\mathbf{d}} - \dot{\Psi} - \varrho_0 \eta \dot{\theta} - \theta^{-1} \boldsymbol{q} \cdot \nabla \theta \geqslant 0. \tag{2.12}$$

Here $\Psi(\boldsymbol{X}, t)$ denotes the free energy function measured per unit volume of the reference configuration

$$\Psi \equiv \varrho_0 \psi = \varrho_0 (\varepsilon - \theta \eta) \tag{2.13}$$

and $\mathscr{D}(\boldsymbol{X}, t)$ is the dissipation function.

2.4. General constitutive equations for damage process in thermo-viscoelastic material

Within the present micromechanical damage theory, the independent thermo-kinetic field variables are $(\boldsymbol{x}, \mathbf{d}, \theta)$ corresponding to $(\boldsymbol{x}, \mathbf{F}^p, \theta)$ in a Lagrangean description of finite elastoplasticity (e.g. Schieck et al., 1999). They must be determined as solution of the problem. The unknown dependent field variables are $(\Psi, \boldsymbol{T}, \mathbf{k}, \mathbf{H}, \eta, \boldsymbol{q})$, which must be given by constitutive equations in terms of the independent field variables $(\boldsymbol{x}, \mathbf{d}, \theta)$. For thermo-viscoelastic damage, we assume the constitutive equations in the general form

$$\begin{aligned} &\Psi = \widehat{\Psi}(\mathbb{e}, \mathbb{f}, \nabla\theta), \quad \boldsymbol{T} = \widehat{\boldsymbol{T}}(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ &\mathbf{k} = \hat{\mathbf{k}}(\mathbb{e}, \mathbb{f}, \nabla\theta), \quad \mathbf{H} = \widehat{\mathbf{H}}(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ &\eta = \hat{\eta}(\mathbb{e}, \mathbb{f}, \nabla\theta), \quad \boldsymbol{q} = \hat{\boldsymbol{q}}(\mathbb{e}, \mathbb{f}, \nabla\theta), \end{aligned} \tag{2.14}$$

with the shortenings $\mathbb{e} = (\boldsymbol{F}, \mathbf{d}, \nabla\mathbf{d}, \theta)$ and $\mathbb{f} = (\dot{\boldsymbol{F}}, \dot{\mathbf{d}}, \Delta\dot{\mathbf{d}})$.

The general constitutive equations (2.14) must be consistent with the balance law of angular momentum $(2.7)_2$ and the reduced dissipation inequality (2.12). Introducing the constitutive equations (2.14) into (2.12) yields

$$\begin{aligned} \mathscr{D} = {} & (\widehat{\boldsymbol{T}} - \partial_{\boldsymbol{F}} \widehat{\Psi}) \cdot \dot{\boldsymbol{F}} + (\hat{\mathbf{k}} - \partial_{\mathbf{d}} \widehat{\Psi}) \cdot \dot{\mathbf{d}} + (\widehat{\mathbf{H}} - \partial_{\nabla\mathbf{d}} \widehat{\Psi}) \cdot \nabla\dot{\mathbf{d}} \\ & - (\varrho_0 \hat{\eta} + \partial_\theta \widehat{\Psi}) \dot{\theta} - \theta^{-1} \hat{\boldsymbol{q}} \cdot \nabla\theta - \partial_{\dot{\boldsymbol{F}}} \widehat{\Psi} \cdot \ddot{\boldsymbol{F}} - \partial_{\dot{\mathbf{d}}} \widehat{\Psi} \cdot \ddot{\mathbf{d}} - \partial_{\nabla\dot{\mathbf{d}}} \widehat{\Psi} \cdot \nabla\ddot{\mathbf{d}} - (\partial_{\nabla\theta} \widehat{\Psi}) \cdot \nabla\dot{\theta} \geqslant 0. \end{aligned} \tag{2.15}$$

Since the inequality (2.15) must be satisfied identically by all constitutive functions, it follows that

$$\partial_{\dot{\boldsymbol{F}}} \widehat{\Psi} = \mathbf{0}, \quad \partial_{\dot{\mathbf{d}}} \widehat{\Psi} = \mathbf{0}, \quad \partial_{\nabla\dot{\mathbf{d}}} \widehat{\Psi} = \mathbf{0}, \quad \partial_{\nabla\theta} \widehat{\Psi} = \mathbf{0}. \tag{2.16}$$

Thus the free energy density Ψ depends neither on the time derivative of the deformation gradient, $\dot{\boldsymbol{F}}$, of the damage variable and its gradient, $\dot{\mathbf{d}}$, $\nabla\dot{\mathbf{d}}$, nor on the temperature gradient $\nabla\theta$. Hence

$$\Psi = \widehat{\Psi}(\mathbb{e}) = \widehat{\Psi}(\boldsymbol{F}, \mathbf{d}, \nabla\mathbf{d}, \theta). \tag{2.17}$$

Moreover, from (2.15) it follows that the entropy η is determined by the constitutive equation of the free energy:

$$\varrho_0 \eta = \varrho_0 \hat{\eta}(\mathbb{e}) = -\partial_\theta \widehat{\Psi}(\mathbb{e}). \tag{2.18}$$

Furthermore, as a consequence of inequality (2.15) we obtain also the result that the first Piola–Kirchhoff stress tensor $\boldsymbol{T}$, the microforce vector $\mathbf{k}$ and the microstress tensor $\mathbf{H}$ consist of two contributions, a non-dissipative and a dissipative one

$$\begin{aligned} &\boldsymbol{T} = \widehat{\boldsymbol{T}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\boldsymbol{F}} \widehat{\Psi}(\mathbb{e}) + \widehat{\boldsymbol{T}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ &\mathbf{k} = \hat{\mathbf{k}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\mathbf{d}} \widehat{\Psi}(\mathbb{e}) + \hat{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ &\mathbf{H} = \widehat{\mathbf{H}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\nabla\mathbf{d}} \widehat{\Psi}(\mathbb{e}) + \widehat{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta). \end{aligned} \tag{2.19}$$

As it is seen the non-dissipative parts are determined by the constitutive form of the free energy function $\widehat{\Psi}(\mathbb{e})$, while the dissipative parts, denoted by a lower asterisk, must be specified independently for each class of material. In general, they must satisfy the reduced dissipation inequality

$$\mathscr{D} = \widehat{\boldsymbol{T}}_* \cdot \dot{\boldsymbol{F}} + \hat{\mathbf{k}}_* \cdot \dot{\mathbf{d}} + \widehat{\mathbf{H}}_* \cdot \nabla\dot{\mathbf{d}} - \theta^{-1}\hat{\boldsymbol{q}} \cdot \nabla\theta \geqslant 0. \tag{2.20}$$

In (2.20) the first term represents the dissipation due to the driving macroforce, the second and third term the dissipation due to evolving microdefects, and the fourth term the dissipation due to heat transfer.

Constitutive equations of the form (2.19), in less general form, were presented in Le and Stumpf (1996) for finite elastoplasticity taking into account the dislocation motion. There, $\boldsymbol{F}^p$ and $\nabla\boldsymbol{F}^p$, representing dislocations, correspond to $\mathbf{d}$ and $\nabla\mathbf{d}$ in the present micromechanical damage model.

The possible forms of the response functions (2.17)–(2.19) are further restricted by the principle of frame-indifference. The simplest way to obtain frame-indifferent constitutive equations is to choose the second Piola–Kirchoff stress tensor $\boldsymbol{S}$ and the Green strain tensor $\boldsymbol{E}$ instead of $\boldsymbol{T}$ and $\boldsymbol{F}$. Assuming also the damage variables $\mathbf{d}(\boldsymbol{X},t)$ in objective form, the standard procedures can be applied to show the frame-indifference of the constitutive equations consisting of

$$\Psi = \widetilde{\Psi}(\mathbb{e}), \quad \mathbb{e} = (\boldsymbol{E}, \mathbf{d}, \nabla\mathbf{d}, \theta) \tag{2.21}$$

together with

$$\begin{aligned} \boldsymbol{S} &= \widetilde{\boldsymbol{S}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\boldsymbol{E}}\widetilde{\Psi}(\mathbb{e}) + \widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ \mathbf{k} &= \tilde{\mathbf{k}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \tilde{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ \mathbf{H} &= \widetilde{\mathbf{H}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\nabla\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \widetilde{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta), \end{aligned} \tag{2.22}$$

where $\mathbb{f} = (\dot{\boldsymbol{E}}, \dot{\mathbf{d}}, \nabla\dot{\mathbf{d}})$, and

$$\varrho_0\eta = \varrho_0\tilde{\eta}(\mathbb{e}) = -\partial_\theta\widetilde{\Psi}(\mathbb{e}), \quad \boldsymbol{q} = \tilde{\boldsymbol{q}}(\mathbb{e}, \mathbb{f}, \nabla\theta). \tag{2.23}$$

With (2.21)–(2.23) the reduced dissipation inequality (2.20) takes the frame invariant form

$$\mathscr{D} = \widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \dot{\boldsymbol{E}} + \tilde{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \dot{\mathbf{d}} + \widetilde{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \nabla\dot{\mathbf{d}} - \theta^{-1}\tilde{\boldsymbol{q}} \cdot \nabla\theta \geqslant 0. \tag{2.24}$$

As it is seen, the complete specification of the constitutive equations requires the determination of the response functions $\widetilde{\Psi}(\mathbb{e})$, $\tilde{\boldsymbol{q}}(\mathbb{e}, \mathbb{f}, \nabla\theta)$, $\widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$, $\tilde{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$ and $\widetilde{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$. In the case of dynamical damage evolution, also the inertia tensor $\mathbf{A}$ of the moving microdefects must be determined by a constitutive equation.

2.5. Dissipation pseudo-potential

The form of the reduced dissipation inequality (2.24) suggests to assume the existence of a dissipation pseudo-potential of the general form

$$\Phi = \widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta) \tag{2.25}$$

such that the dissipative macro- and microforces, microstresses and the heat flux vector can be obtained as

$$\begin{aligned} \widetilde{\boldsymbol{S}}_* &= \partial_{\dot{\boldsymbol{E}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ \tilde{\mathbf{k}}_* &= \partial_{\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ \widetilde{\mathbf{H}}_* &= \partial_{\nabla\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta), \\ \theta^{-1}\boldsymbol{q} &= -\partial_{\nabla\theta}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta). \end{aligned} \tag{2.26}$$

With (2.25) and (2.26) the general constitutive equations for macro- and microforces and microstresses can be given as functions of the free energy potential $\widetilde{\Psi}$ and the dissipation pseudo-potential $\widetilde{\Phi}$

$$\begin{aligned}
&\boldsymbol{S} = \widetilde{\boldsymbol{S}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\boldsymbol{E}}\widetilde{\Psi}(\mathbb{e}) + \partial_{\dot{\boldsymbol{E}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta),\\
&\mathbf{k} = \tilde{\mathbf{k}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \partial_{\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta),\\
&\mathbf{H} = \widetilde{\mathbf{H}}(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\nabla\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \partial_{\nabla\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta),\\
&\theta^{-1}\boldsymbol{q} = -\partial_{\nabla\theta}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta),
\end{aligned} \tag{2.27}$$

while the dissipation inequality (2.24) takes now the form

$$\mathscr{D} = \partial_{\dot{\boldsymbol{E}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)\cdot\dot{\boldsymbol{E}} + \partial_{\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)\cdot\dot{\mathbf{d}} + \partial_{\nabla\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)\cdot\nabla\dot{\mathbf{d}} + \partial_{\nabla\theta}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)\cdot\nabla\theta \geqslant 0. \tag{2.28}$$

The advantage of the introduction of a dissipation pseudo-potential is obvious. Instead of specifying the four response functions $\widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$, $\tilde{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$, $\widetilde{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)$ and $\tilde{\boldsymbol{q}}(\mathbb{e}, \mathbb{f}, \nabla\theta)$ independently, the choice of one scalar-valued response function (2.25) determines completely the dissipative parts of the macro- and microvariables. However, the existence of the dissipation pseudo-potential must be proved for each class of problems.

2.6. Micromechanical damage theory

Introducing the constitutive equations (2.22) into the balance laws of macro- and microforces $(2.7)_1$ and (2.8), taking into account (2.5), the following system of coupled field equations for the analysis of the damage evolution is obtained:

$$\begin{aligned}
&\mathrm{Div}(\boldsymbol{F}\partial_{\boldsymbol{E}}\widetilde{\Psi}(\mathbb{e}) + \boldsymbol{F}\widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)) + \boldsymbol{b} = \varrho_0\ddot{\boldsymbol{x}},\\
&\mathrm{Div}(\partial_{\nabla\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \widetilde{\mathbf{H}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)) - \partial_{\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) - \tilde{\mathbf{k}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) + \mathbf{g} = \varrho_0\mathbf{A}\ddot{\mathbf{d}}
\end{aligned} \tag{2.29}$$

with the arguments $\mathbb{e} = (\boldsymbol{E}, \mathbf{d}, \nabla\mathbf{d}, \theta)$ and $\mathbb{f} = (\dot{\boldsymbol{E}}, \dot{\mathbf{d}}, \nabla\dot{\mathbf{d}})$. If for the problem under consideration there exists a dissipation pseudo-potential $\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)$ such that the constitutive equations (2.27) are valid, the governing equations (2.29) for the damage analysis are obtained as

$$\begin{aligned}
&\mathrm{Div}(\boldsymbol{F}\partial_{\boldsymbol{E}}\widetilde{\Psi}(\mathbb{e}) + \boldsymbol{F}\partial_{\dot{\boldsymbol{E}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)) + \boldsymbol{b} = \varrho_0\ddot{\boldsymbol{x}},\\
&\mathrm{Div}(\partial_{\nabla\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) + \partial_{\nabla\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)) - \partial_{\mathbf{d}}\widetilde{\Psi}(\mathbb{e}) - \partial_{\dot{\mathbf{d}}}\widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta) + \mathbf{g} = \varrho_0\mathbf{A}\ddot{\mathbf{d}}.
\end{aligned} \tag{2.30}$$

Eqs. (2.29) and (2.30), respectively, must be supplemented by appropriate boundary and initial conditions. In the classical macrotheory, the boundary conditions at any point $\boldsymbol{X} \in \partial B_0$ consist of prescribed displacements or tractions or some suitable combination thereof. Here, we assume that there are two disjoint, time independent subsets of ∂B_0 such that the traction boundary condition is specified on the part ∂B_{0f} (analogous to the Neumann condition), while on the complementary part ∂B_{0u} the kinematic boundary condition is specified (analogous to the Dirichlet condition):

$$\begin{aligned}
&\boldsymbol{T}(\boldsymbol{X}, t)\boldsymbol{n}_0(\boldsymbol{X}) = \boldsymbol{t}^*(\boldsymbol{X}, t), \quad (\boldsymbol{X}, t) \in \partial B_{0f} \times T,\\
&\boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{u}^*(\boldsymbol{X}, t), \quad (\boldsymbol{X}, t) \in \partial B_{0u} \times T,
\end{aligned} \tag{2.31}$$

where $\boldsymbol{T} = \boldsymbol{FS}$ and $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X}$. The boundary conditions associated with the damage field $\mathbf{d}$ are formulated in the same manner, i.e. on two complementary parts ∂B_{0k} and $\partial B_{0d} = \partial B_0 \setminus \partial B_{0k}$ of the boundary the following conditions are assumed

$$\begin{aligned}
&\mathbf{H}(\boldsymbol{X}, t)\boldsymbol{n}_0(\boldsymbol{X}) = \mathbf{k}^*(\boldsymbol{X}, t), \quad (\boldsymbol{X}, t) \in \partial B_{0k} \times T,\\
&\mathbf{d}(\boldsymbol{X}, t) = \mathbf{d}^*(\boldsymbol{X}, t), \quad (\boldsymbol{X}, t) \in \partial B_{0d} \times T.
\end{aligned} \tag{2.32}$$

The initial conditions at time $t = 0$ for all $\boldsymbol{X} \in B$ are

$$\begin{aligned} &\boldsymbol{x}(\boldsymbol{X},0) = \boldsymbol{x}_0(\boldsymbol{X}), \quad \dot{\boldsymbol{x}}(\boldsymbol{X},0) = \boldsymbol{v}_0(\boldsymbol{X}), \\ &\mathbf{d}(\boldsymbol{X},0) = \mathbf{d}_0(\boldsymbol{X}), \quad \dot{\mathbf{d}}(\boldsymbol{X},0) = \boldsymbol{v}_0(\boldsymbol{X}). \end{aligned} \tag{2.33}$$

The fields marked in (2.31)–(2.33) by upper asterisks and lower index zero, respectively, are given functions which must be specified for each class of initial-boundary value problems.

The presented Eqs. (2.29)–(2.33) together with the local equation of energy balance (2.9) and appropriate boundary and initial conditions for temperature and heat flux constitute the complete set of field equations and initial and boundary conditions to define a damage evolution theory for thermo-viscoelastic bodies subject to arbitrary dynamical loading. It provides a thermodynamically consistent framework for the modeling of weakly nonlocal as well as local damage theories for thermo-viscoelastic and quasi-brittle materials.

Simplifications of the general result are obtained by assuming

- quasi-static deformation and quasi-static damage evolution: $\ddot{\boldsymbol{x}} = \mathbf{0}$, $\mathbf{A}\ddot{\mathbf{d}} = \mathbf{0}$,
- no chemical reactions breaking internal material bonds: $\mathbf{g} = 0$,
- isothermal process: $\nabla\theta = \mathbf{0}$, $\theta(\boldsymbol{X},t) = \text{const.}$,
- isotropic damage described by a single scalar-valued damage parameter: $\mathbf{d} = (d,0,0)$.

Because of its importance for engineering applications the case of isotropic damage will be considered in the following section for various classes of material properties. Analogous results can be derived also for anisotropic damage (see Section 4.1).

3. Isotropic damage

3.1. Thermo-viscoelastic material

In the case of isotropic damage the process of degradation of material is described by a single scalar-valued function $d(\boldsymbol{X},t)$ and its gradient by the vector-valued function $\nabla d(\boldsymbol{X},t) \in E$, where d may represent e.g. the number of microcracks in a representative volume element and ∇d is its spatial change. In this case the balance law of microforces (2.8) with $(2.5)_2$ reduces to the balance equation of scalar-valued microforces

$$\mathrm{Div}\boldsymbol{h} - k + g = \varrho_0 A\ddot{d}. \tag{3.1}$$

Here $\boldsymbol{h}(\boldsymbol{X},t) \in E$ is the microstress vector work-conjugate to ∇d, $k(\boldsymbol{X},t)$ a scalar-valued microforce work-conjugate to d, $g(\boldsymbol{X},t)$ a scalar-valued chemical reaction, and $A(\boldsymbol{X})$ the microinertia coefficient associated with the dynamical microcrack evolution. It should be noted that the time-scale of chemical reactions is in general quite different from the time-scale of the thermodynamical process of damage.

With the shortenings $\mathbb{e} = (\boldsymbol{E}, d, \nabla d, \theta)$ and $\mathbb{f} = (\dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$, the free energy is given by a free energy function $\Psi = \widetilde{\Psi}(\mathbb{e})$, and the constitutive equations (2.22) and (2.23) reduce to the form

$$\begin{aligned} &\boldsymbol{S} = \partial_{\boldsymbol{E}}\widetilde{\Psi}(\mathbb{e}) + \widetilde{\boldsymbol{S}}_*(\mathbb{e},\mathbb{f},\nabla\theta), \\ &k = \partial_d\widetilde{\Psi}(\mathbb{e}) + \tilde{k}_*(\mathbb{e},\mathbb{f},\nabla\theta), \\ &\boldsymbol{h} = \partial_{\nabla d}\widetilde{\Psi}(\mathbb{e}) + \tilde{\boldsymbol{h}}_*(\mathbb{e},\mathbb{f},\nabla\theta) \end{aligned} \tag{3.2}$$

and

$$\varrho_0\eta = \varrho_0\tilde{\eta}(\mathbb{e}) = -\partial_\theta\widetilde{\Psi}(\mathbb{e}), \quad \boldsymbol{q} = \tilde{\boldsymbol{q}}(\mathbb{e},\mathbb{f},\nabla\theta). \tag{3.3}$$

If there exists a dissipation pseudo-potential $\Phi = \widetilde{\Phi}(\mathbb{e}, \mathbb{f}, \nabla\theta)$, then the dissipative parts of the constitutive equations (3.2) are given by

$$\begin{aligned} &\widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\dot{\boldsymbol{E}}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta),\\ &\tilde{k}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\dot{d}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta),\\ &\tilde{\boldsymbol{h}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) = \partial_{\nabla\dot{d}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta) \end{aligned} \tag{3.4}$$

and $(3.3)_2$ by

$$\theta^{-1}\boldsymbol{q} = -\partial_{\nabla\theta}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta). \tag{3.5}$$

The dissipation inequality (2.24) reads for isotropic damage

$$\mathscr{D} = \widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \dot{\boldsymbol{E}} + \tilde{k}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)\dot{d} + \tilde{\boldsymbol{h}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \nabla\dot{d} - \tilde{\boldsymbol{q}}(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \nabla\theta \geqslant 0 \tag{3.6}$$

and

$$\mathscr{D} = \partial_{\dot{\boldsymbol{E}}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \dot{\boldsymbol{E}} + \partial_{\dot{d}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta)\dot{d} + \partial_{\nabla\dot{d}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \nabla\dot{d} + \partial_{\nabla\theta}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}, \nabla\theta) \cdot \nabla\theta \geqslant 0, \tag{3.7}$$

respectively.

The macro- and microbalance laws for isotropic damage evolution in thermo-viscoelastic material follow from (2.29) as

$$\begin{aligned} &\mathrm{Div}(\boldsymbol{F}\partial_{\boldsymbol{E}}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \boldsymbol{F}\tilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)) + \boldsymbol{b} = \varrho_0\ddot{\boldsymbol{x}},\\ &\mathrm{Div}(\partial_{\nabla d}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \tilde{\boldsymbol{h}}_*(\mathbb{e}, \mathbb{f}, \nabla\theta)) - \partial_d\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) - \tilde{k}_*(\mathbb{e}, \mathbb{f}, \nabla\theta) + g = \varrho_0 A\ddot{d} \end{aligned} \tag{3.8}$$

and corresponding equations, if the constitutive relations (3.4) are valid.

3.2. Isothermal process

3.2.1. Quasi-brittle and elastic materials

For isothermal process the space gradient of temperature vanishes, $\nabla\theta = \boldsymbol{0}$. Consequently, the heat flux vector vanishes according to (3.5), $\boldsymbol{q} = \boldsymbol{0}$, and the constitutive equations (3.2) reduce to the form

$$\boldsymbol{S} = \partial_{\boldsymbol{E}}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \tilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}), \quad k = \partial_d\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \tilde{k}_*(\mathbb{e}, \mathbb{f}), \quad \boldsymbol{h} = \partial_{\nabla d}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \tilde{\boldsymbol{h}}_*(\mathbb{e}, \mathbb{f}) \tag{3.9}$$

with $\mathbb{e} \equiv (\boldsymbol{E}, d, \Delta d)$ and $\mathbb{f} \equiv (\dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$. These constitutive equations include rate effects of the macrostrains and of the damage variables. However, in the damage analysis of quasi-brittle materials such as concrete and ceramics rate effects can often be neglected so that further simplifications of the constitutive equations (3.9) are possible.

We assume that the dissipative parts of the second Piola–Kirchhoff stress tensor, $\tilde{\boldsymbol{S}}_*$, and of the micro-stress vector, $\tilde{\boldsymbol{h}}_*$, are small and can be neglected:

$$\widetilde{\boldsymbol{S}}_*(\mathbb{e}, \mathbb{f}) = \partial_{\dot{\boldsymbol{E}}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}) = \boldsymbol{0}, \quad \tilde{\boldsymbol{h}}_*(\mathbb{e}, \mathbb{f}) = \partial_{\nabla\dot{d}}\widetilde{\boldsymbol{\Phi}}(\mathbb{e}, \mathbb{f}) = \boldsymbol{0}, \tag{3.10}$$

leading to the constitutive equations

$$\boldsymbol{S} = \partial_{\boldsymbol{E}}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}), \quad \boldsymbol{h} = \partial_{\nabla d}\widetilde{\boldsymbol{\Psi}}(\mathbb{e}). \tag{3.11}$$

However, even for quasi-brittle material we cannot neglect the dissipative part of the intrinsic microforce k. Thus, with $(3.9)_2$ we have

$$k = \partial_d\widetilde{\boldsymbol{\Psi}}(\mathbb{e}) + \tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}). \tag{3.12}$$

Then, the dissipation inequality (3.6) reduces to the form

$$\mathscr{D} = \tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})\dot{d} \geqslant 0. \tag{3.13}$$

From (3.13) the following general restriction for the dissipative part of the intrinsic microforce is obtained:

$$\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}) \geqslant 0, \tag{3.14}$$

whenever $\dot{d} > 0$, i.e. the damage increases. The case $\dot{d} < 0$ is considered to be physically not realistic.

If there exists a dissipation pseudo-potential $\Phi = \widetilde{\Phi}(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$ such that

$$\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}) = \partial_{\dot{d}}\widetilde{\Phi}(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}), \tag{3.15}$$

then the dissipation inequality (3.13) takes the form

$$\mathscr{D} = \partial_{\dot{d}}\widetilde{\Phi}(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})\dot{d} \geqslant 0. \tag{3.16}$$

The restrictions (3.14) and (3.16), respectively, are direct consequences of the reduced dissipation inequality, which in turn was derived as implication of the Clausius–Duhem inequality (2.12).

A further specification can be obtained, if we assume that the driving microforce $\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$ for quasi-brittle and elastic material is homogeneous of degree one with respect to $\dot{\boldsymbol{E}}$, $\dot{d}$ and $\nabla\dot{d}$. Hence, its general form can be written as

$$\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}) = \mathscr{B}(\mathbb{e}) - \mathscr{C}(\mathbb{e})\dot{d} + \boldsymbol{L}(\mathbb{e}) \cdot \dot{\boldsymbol{E}} + \mathscr{H}(\mathbb{e}) \cdot \nabla\dot{d}. \tag{3.17}$$

Here, $\mathscr{B}(\mathbb{e})$, $\mathscr{C}(\mathbb{e})$ are scalar-valued, $\mathscr{H}(\mathbb{e})$ vector-valued, and $\boldsymbol{L}(\mathbb{e})$ tensor-valued functions of $\mathbb{e} \equiv (\boldsymbol{E}, d, \nabla d)$. With (3.17) the constitutive equation (3.12) for intrinsic microforce takes the form

$$k = \partial_d\widetilde{\Psi}(\mathbb{e}) + \mathscr{B}(\mathbb{e}) - \mathscr{C}(\mathbb{e})\dot{d} + \boldsymbol{L}(\mathbb{e}) \cdot \dot{\boldsymbol{E}} + \mathscr{H}(\mathbb{e}) \cdot \nabla\dot{d}. \tag{3.18}$$

A slightly different, but for later considerations appropriate constitutive form of the microforce k is obtained by assuming that instead of its dissipative part (3.17) $\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$ can be represented as

$$\tilde{k}_*(\mathbb{e}, \dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d}) = \mathscr{B}(\mathbb{e}) - \mathscr{C}(\mathbb{e})\dot{d} + \mathscr{L}(\mathbb{e})\dot{\mathscr{E}}(\boldsymbol{E}) + \mathscr{H}(\mathbb{e}) \cdot \nabla\dot{d} \tag{3.19}$$

with $\mathscr{L}$ and $\mathscr{E}$ scalar-valued constitutive functions. Then, the microforce (3.18) takes the form

$$k = -\mathscr{C}(\mathbb{e})\dot{d} + \mathscr{L}(\mathbb{e})\dot{\mathscr{E}}(\boldsymbol{E}) + \mathscr{H}(\mathbb{e}) \cdot \nabla\dot{d} + \mathscr{W}(\mathbb{e}) \tag{3.20}$$

with

$$\mathscr{W}(\mathbb{e}) \equiv \partial_d\widetilde{\Psi}(\mathbb{e}) + \mathscr{B}(\mathbb{e}). \tag{3.21}$$

Assuming that $\mathscr{E} = \mathscr{E}(\boldsymbol{E})$ is differentiable, then $\dot{\mathscr{E}}(\boldsymbol{E}) = \partial_{\boldsymbol{E}}\mathscr{E}(\boldsymbol{E}) \cdot \dot{\boldsymbol{E}}$ and hence

$$\mathscr{L}(\mathbb{e})\dot{\mathscr{E}}(\boldsymbol{E}) = \mathscr{L}(\mathbb{e})\partial_{\boldsymbol{E}}\mathscr{E}(\boldsymbol{E}) \cdot \dot{\boldsymbol{E}}. \tag{3.22}$$

A comparison of (3.17) with (3.19) leads to the representation $\boldsymbol{L}(\mathbb{e}) = \mathscr{L}(\mathbb{e})\partial_{\boldsymbol{E}}\mathscr{E}(\boldsymbol{E})$, which is used in the next section to specify the microforce k.

3.2.2. Isotropic elastic material

If the material possesses some symmetries in its physical structure further specifications of the constitutive response functions are possible. Such properties are defined in terms of material symmetry groups (Truesdell and Noll, 1965). For isotropic material, the symmetry group is the full orthogonal group $\mathrm{O}(E)$. In this case, the combined restrictions due to material frame-indifference and material symmetry imply that the free energy response function $\widetilde{\Psi}(\boldsymbol{E}, d, \nabla d)$ is an isotropic function of its arguments. Accordingly, by the classical representation theorem of tensor functions (e.g. Truesdell and Noll, 1965), $\widetilde{\Psi}(\mathbb{e}) = \widetilde{\Psi}(\boldsymbol{E}, d, \nabla d)$

depends on $\boldsymbol{E}$ and ∇d only through the joint invariants of $\boldsymbol{E}$ and ∇d consisting of three principal invariants I_1, I_2, I_3 of $\boldsymbol{E}$ defined by

$$I_1 = \mathrm{tr}E, \quad I_2 = \frac{1}{2}\{(\mathrm{tr}\boldsymbol{E})^2 - \mathrm{tr}(\boldsymbol{E}^2)\}, \quad I_3 = \det \boldsymbol{E} \tag{3.23}$$

and three additional joint invariants I_4, I_5, I_6 defined by

$$I_4 = \nabla d \cdot \nabla d, \quad I_5 = \nabla d \cdot \boldsymbol{E}\nabla d, \quad I_6 = \nabla d \cdot \boldsymbol{E}^2 \nabla d. \tag{3.24}$$

Thus, the constitutive form of the free energy $\Psi = \widetilde{\Psi}(\boldsymbol{E}, d, \nabla d)$ for finite strains $\boldsymbol{E}$ and arbitrary vectors ∇d is

$$\Psi = \widetilde{\Psi}(d, \mathbb{i}, \mathbb{j}), \quad \mathbb{i} \equiv (I_1, I_2, I_3), \quad \mathbb{j} \equiv (I_4, I_5, I_6), \tag{3.25}$$

leading with (3.11) to the constitutive equations for the stress tensor $\boldsymbol{S}$ and the microstress vector $\boldsymbol{h}$

$$\boldsymbol{S} = (W_1 + I_1 W_2 + I_2 W_3)\mathbf{1} + (W_2 - I_1 W_3)\boldsymbol{E} + W_3 \boldsymbol{E}^2 + W_5(\nabla d \otimes \nabla d) + W_6(\boldsymbol{E}\nabla d \otimes \nabla d + \nabla d \otimes \boldsymbol{E}\nabla d) \tag{3.26}$$

and

$$\boldsymbol{h} = 2(W_4 \mathbf{1} + W_5 \boldsymbol{E} + W_6 \boldsymbol{E}^2)\Delta d, \tag{3.27}$$

where

$$W_\alpha = W_\alpha(d, \mathbb{i}, \mathbb{j}) \equiv \partial \widetilde{\Psi}(d, \mathbb{i}, \mathbb{j}) / \partial I_\alpha, \quad \alpha = 1, \ldots, 6. \tag{3.28}$$

The constitutive equation for the microforce k according to (3.20) and (3.21) is obtained as

$$k = -\mathscr{C}(d, \mathbb{i}, \mathbb{j})\dot{d} + \mathscr{L}(d, \mathbb{i}, \mathbb{j})\dot{\mathscr{E}}(\mathbb{i}) + \mathscr{H}(d, \mathbb{i}, \mathbb{j}) \cdot \nabla \dot{d} + \mathscr{W}(d, \mathbb{i}, \mathbb{j}) \tag{3.29}$$

with

$$\mathscr{W}(d, \mathbb{i}, \mathbb{j}) \equiv \partial_d \widetilde{\Psi}(d, \mathbb{i}, \mathbb{j}) + \mathscr{B}(d, \mathbb{i}, \mathbb{j}), \tag{3.30}$$

where $\mathbb{i}$ and $\mathbb{j}$ stand for the lists of invariants defined in (3.25). Moreover, the time derivative of $\mathscr{E} = \mathscr{E}(\mathbb{i})$ is given by

$$\dot{\mathscr{E}} = (\partial_{I_1}\mathscr{E})\dot{I}_1 + (\partial_{I_2}\mathscr{E})\dot{I}_2 + (\partial_{I_3}\mathscr{E})\dot{I}_3. \tag{3.31}$$

Noting that the invariants $\mathbb{i} \equiv (I_1, I_2, I_3)$ are defined by (3.23) it is not difficult to show that

$$\dot{I}_1 = \mathbf{1} \cdot \dot{\boldsymbol{E}}, \quad \dot{I}_2 = (I_1\mathbf{1} - \boldsymbol{E}) \cdot \dot{\boldsymbol{E}}, \quad \dot{I}_3 = (I_2\mathbf{1} - I_1\boldsymbol{E} + \boldsymbol{E}^2) \cdot \dot{\boldsymbol{E}}. \tag{3.32}$$

Substituting (3.32) into (3.31) yields

$$\dot{\mathscr{E}} = \{(E_1 + I_1 E_2 + I_2 E_3)\mathbf{1} - (E_2 + I_1 E_3)\boldsymbol{E} + E_3 \boldsymbol{E}^2\} \cdot \dot{\boldsymbol{E}}, \tag{3.33}$$

where $E_k = \partial\mathscr{E}/\partial I_k$, $k = 1, 2, 3$.

Similar relations can be derived also if the dissipative part of the microforce $\tilde{k}_*$ according to (3.19) is given in terms of a pseudo-dissipation potential.

3.2.3. Application of the strain equivalence hypothesis

Essential simplifications of the constitutive equations are obtained by assuming a specific form of the free energy function $\widetilde{\Psi}(\boldsymbol{E}, d, \nabla d)$ and $\Psi(d, \mathbb{i}, \mathbb{j})$, respectively. A simple model of this kind, which nevertheless encompasses a wide class of brittle materials, is described by a free energy function of the form

$$\Psi = \widetilde{\Psi}(\boldsymbol{E}, d, \nabla d) = (1 - d)\Psi^0(\boldsymbol{E}) + \bar{\Psi}(\nabla d), \tag{3.34}$$

where $\Psi^0(\boldsymbol{E})$ is identified with the free energy of the undamaged elastic material, and $\bar{\Psi}(\nabla d)$ represents that contribution to the free energy resulting from weakly non-local interactions. The assumption (3.34), which can be regarded as a weakly non-local generalization of the so-called strain equivalence hypothesis, yields the constitutive equations for the stress tensor $\boldsymbol{S}$ and the microforce vector $\boldsymbol{h}$ according to (3.11) in the form

$$\boldsymbol{S} = (1-d)\partial_{\boldsymbol{E}}\Psi^0(\boldsymbol{E}), \quad \boldsymbol{h} = \partial_{\nabla d}\bar{\Psi}(\nabla d). \tag{3.35}$$

Assuming that in (3.20) the term $\mathscr{H}(\mathbb{e})\cdot\nabla\dot{d}$ can be neglected the microforce k is obtained as

$$k = -\mathscr{C}(\mathbb{e})\dot{d} + \mathscr{L}(\mathbb{e})\dot{\mathscr{E}}(\boldsymbol{E}) + \mathscr{W}(\mathbb{e}) \tag{3.36}$$

with

$$\mathscr{W}(\mathbb{e}) = -\Psi^0(\boldsymbol{E}) + \mathscr{B}(\mathbb{e}) \tag{3.37}$$

and $\mathbb{e} \equiv (\boldsymbol{E}, d, \nabla d)$.

For isotropic elastic material behavior, Ψ^0 and $\bar{\Psi}$ and the constitutive functions appearing in (3.36) must be isotropic functions of their arguments. Thus

$$\Psi^0 = \Psi^0(I_1, I_2, I_3), \quad \bar{\Psi} = \Psi(I_4), \tag{3.38}$$

where the invariants are defined by (3.23) and $(3.24)_1$. From (3.26) and (3.27), it follows that in the case of isotropic material behavior the constitutive equations (3.35) reduce to the form

$$\boldsymbol{S} = (1-d)(W_1^0 + I_1 W_2^0 + I_2 W_3^0)\mathbf{1} + (W_2^0 - I_1 W_3^0)\boldsymbol{E} + W_3^0\boldsymbol{E}^2 \tag{3.39}$$

and

$$\boldsymbol{h} = \partial_{\nabla d}\bar{\Psi}(\nabla d) = 2\overline{W}_4\mathbf{1}\nabla d, \tag{3.40}$$

where

$$W_i^0 \equiv \partial\Psi^0(I_1, I_2, I_3)/\partial I_i, \quad i = 1,2,3, \quad \overline{W}_4 \equiv \partial\bar{\Psi}(I_4)/\partial I_4. \tag{3.41}$$

Moreover, the constitutive equation (3.36) takes the form

$$k = -\mathscr{C}(d, \mathbb{i}, \mathbb{j})\dot{d} + \mathscr{L}(d, \mathbb{i}, \mathbb{j})\dot{\mathscr{E}}(\mathbb{i}) + \mathscr{W}(d, \mathbb{i}, \mathbb{j}) \tag{3.42}$$

with

$$\mathscr{W}(d, \mathbb{i}, \mathbb{j}) = -\Psi^0(I_1, I_2, I_3) + \mathscr{B}(d, \mathbb{i}, \mathbb{j}). \tag{3.43}$$

3.2.4. Small strain assumption

Under the assumption of small strains the free energy of the undamaged material Ψ^0 is given by the quadratic form

$$\Psi^0(\boldsymbol{E}) = \frac{1}{2}\{2\mu\,\mathrm{tr}(\boldsymbol{E}^2) + \lambda(\mathrm{tr}\boldsymbol{E})^2\} \tag{3.44}$$

with the Lamé coefficients λ and μ, and the Green strain tensor $\boldsymbol{E}$, which for small strains can be identified also with the linear strain tensor. In (3.38), the invariant $\overline{W}_4$ according to $(3.41)_2$ is constant leading to the weakly non-local energy contribution

$$\bar{\Psi}(\nabla d) = \frac{1}{2}K\nabla d\cdot\nabla d \tag{3.45}$$

and the constitutive equations for the second Piola–Kirchhoff stress tensor $\boldsymbol{S}$ and the microstress vector $\boldsymbol{h}$

$$\boldsymbol{S} = (1-d)\{2\mu\boldsymbol{E} + \lambda(\mathrm{tr}\boldsymbol{E})\mathbf{1}\}, \quad \boldsymbol{h} = K\nabla d. \tag{3.46}$$

For small strains essential simplifications can also be introduced in the constitutive equation for the microforce k due to (3.42). We may assume that $\mathscr{C}$ is independent of ∇d, that $\mathscr{L}$ depends on $\boldsymbol{E}$ only through $\mathscr{E}(\boldsymbol{E})$, and that $\mathscr{E}(\boldsymbol{E})$ and $\mathscr{B}(\boldsymbol{E})$ are independent of ∇d:

$$\mathscr{C}(d,\boldsymbol{E}) \geqslant 0, \quad \mathscr{L}(d,\boldsymbol{E}) = \mathscr{L}(d,\mathscr{E}(\boldsymbol{E})), \quad \mathscr{B} = \mathscr{B}(d,\boldsymbol{E}). \tag{3.47}$$

Then the constitutive equation (3.42) with (3.43) reduces to the form

$$k = -\mathscr{C}(d,\boldsymbol{E})\dot{d} + \mathscr{L}(d,\boldsymbol{E})\dot{\mathscr{E}}(\boldsymbol{E}) + \mathscr{W}(d,\boldsymbol{E}) \tag{3.48}$$

with

$$\mathscr{W}(d,\boldsymbol{E}) = -\Psi^0(\boldsymbol{E}) + \mathscr{B}(d,\boldsymbol{E}). \tag{3.49}$$

For isothermal process with $\nabla\theta = \mathbf{0}$ and isotropic elastic material behavior and applying the strain equivalence hypothesis the balance laws of macro- and microforces (3.8) lead to

$$\begin{aligned} &\mathrm{Div}(\boldsymbol{FS}) + \boldsymbol{b} = \varrho_0\ddot{\boldsymbol{x}}, \\ &Div\boldsymbol{h} - k + g = \varrho_0 A\ddot{d} \end{aligned} \tag{3.50}$$

with the constitutive equations for $\boldsymbol{S}$, $\boldsymbol{h}$ and k given by (3.46)–(3.49) and an additional constitutive equation for the scalar-valued inertia function A. Together with corresponding boundary and initial condition equations (3.50) define a weakly nonlocal and gradient, respectively, model for isotropic damage valid under the assumptions specified above. To construct a FE solution algorithm, we have to formulate a virtual work principle as weak solution of (3.50).

The gradient damage model of Frémond and Nedjar (1996) and Pires-Domingues et al. (1999) is obtained from Eqs. (3.50) and their weak form, if the damage evolution is quasi-static, $\ddot{\boldsymbol{x}} = \mathbf{0}$, $\ddot{d} = 0$, chemical reactions can be neglected, $g = 0$, and the following additional constitutive assumptions are valid:

- $\mathscr{C}(d,\boldsymbol{E}) = C > 0$ is a constant,
- $\mathscr{L}(d,\boldsymbol{E}) = 0$,
- $\mathscr{W}(d,\boldsymbol{E}) = W$ is a constant,

yielding an isotropic damage model with five and six, respectively, material parameters, μ, λ, K, C and W determined experimentally for concrete by Frémond and Nedjar (1996).

4. Anisotropic damage

4.1. One-field modeling

In Section 2 we introduced a set $\mathbf{d} = (d, \boldsymbol{d}, \boldsymbol{D})$ of scalar-, vector- and tensor-valued functions to describe damage phenomena. In this subsection, it is assumed that anisotropic damage can be defined by an anisotropy tensor $\boldsymbol{D}$

$$\mathbf{d} = (0, \mathbf{0}, \boldsymbol{D}). \tag{4.1}$$

In this case, the derivation of anisotropic damage theories can follow the specification and simplification procedure outlined in detail in Section 3 for isotropic damage, so we do not need to repeat it here.

In the literature a one-field anisotropic gradient damage model is proposed by Marshall et al. (1991), where the anisotropy of damage is described by a vector-valued function. In effect, the theory of Marshall et al. follows from the general theory of Section 2 as special case, if we choose $\mathbf{d} = (0, \boldsymbol{d}, \mathbf{0})$.

4.2. Two-field modeling

In this subsection, we assume that anisotropic damage phenomena can be described by a scalar d and a tensor $\boldsymbol{D}$, so that the set of damage variables introduced in Section 2 is

$$\mathbf{d} = (d, \mathbf{0}, \boldsymbol{D}) \tag{4.2}$$

with the gradients

$$\nabla \mathbf{d} = (\nabla d, \mathbf{0}, \nabla \boldsymbol{D}). \tag{4.3}$$

Assuming for simplicity quasi-static isothermal processes the balance law of macroforces follows from $(2.7)_1$ as

$$\mathrm{Div}(\boldsymbol{F}\boldsymbol{S}) + \boldsymbol{b} = \mathbf{0} \tag{4.4}$$

and the balance laws of microforces from (2.8) as

$$\mathrm{Div}\boldsymbol{h} - k + g = 0, \tag{4.5}$$

$$\mathrm{Div}\mathscr{H} - \boldsymbol{K} + \boldsymbol{G} = \mathbf{0}, \tag{4.6}$$

where the microforce k is power-conjugate to $\dot{d}$, $\boldsymbol{K}$ power-conjugate to $\dot{\boldsymbol{D}}$, and the microstresses $\boldsymbol{h}$ and $\mathscr{H}$ power-conjugate to $\nabla\dot{d}$ and $\nabla\dot{\boldsymbol{D}}$, respectively.

For many damage problems of engineering interest, it can be assumed that the gradient of the anisotropy tensor $\boldsymbol{D}$ is small and can be omitted in the list of constitutive variables. Thus, under the assumption $\nabla\boldsymbol{D} = \mathbf{0}$, we have $\mathscr{H} = \mathbf{0}$ so that Eq. (4.6) reduces to the form

$$-\boldsymbol{K} + \boldsymbol{G} = \mathbf{0}. \tag{4.7}$$

Moreover, the free energy (2.21) satisfying the dissipation inequality (2.15) is given by

$$\Psi = \widehat{\Psi}(\mathbb{e}, \boldsymbol{D}), \quad \mathbb{e} = (\boldsymbol{E}, d, \nabla d) \tag{4.8}$$

and the constitutive equations for macrostress $\boldsymbol{S}$, microforces k and $\boldsymbol{K}$, and microstress $\boldsymbol{h}$ by

$$\begin{aligned}
\boldsymbol{S} &= \partial_{\boldsymbol{E}}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + \boldsymbol{S}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}),\\
k &= \partial_d\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + k_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}),\\
\boldsymbol{K} &= \partial_{\boldsymbol{D}}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + \boldsymbol{K}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}),\\
\boldsymbol{h} &= \partial_{\nabla d}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + \boldsymbol{h}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}).
\end{aligned} \tag{4.9}$$

Here $\dot{\mathbb{e}} = (\dot{\boldsymbol{E}}, \dot{d}, \nabla\dot{d})$. The dissipation inequality (2.24) takes now the form

$$\mathscr{D} = \boldsymbol{S}_* \cdot \dot{\boldsymbol{E}} + k_*\dot{d} + \boldsymbol{h}_* \cdot \nabla\dot{d} + \boldsymbol{K} \cdot \dot{\boldsymbol{D}} \geqslant 0. \tag{4.10}$$

Introducing the constitutive equations (4.9) into (4.4)–(4.6), we obtain the governing equations for quasi-static deformation and two-field anisotropic damage evolution

$$\mathrm{Div}(\boldsymbol{F}\partial_{\boldsymbol{E}}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + \boldsymbol{F}\boldsymbol{S}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}})) + \boldsymbol{b} = \mathbf{0}, \tag{4.11}$$

$$\mathrm{Div}(\partial_{\nabla d}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) + \boldsymbol{h}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}})) - \partial_d\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) - k_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}) + g = 0, \tag{4.12}$$

$$-\partial_{\boldsymbol{D}}\widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) - \boldsymbol{K}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}) + \boldsymbol{G} = \mathbf{0}. \tag{4.13}$$

It should be noted that (4.11) and (4.12) are partial differential equations, while (4.13) is an ordinary differential equation. This simplification was obtained by omitting $\nabla \boldsymbol{D}$ in the list of arguments of the constitutive equations. In effect, Eq. (4.13) represents the damage evolution law for $\boldsymbol{D}$ in implicit form.

Assuming that the microforce $\boldsymbol{K}_*$ power-conjugate to $\dot{\boldsymbol{D}}$ is homogeneous of first degree in $\dot{\boldsymbol{D}}$, we can write

$$\boldsymbol{K}_*(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}, \dot{\boldsymbol{D}}) = \mathbb{A}(\mathbb{e}, \boldsymbol{D})\dot{\boldsymbol{D}} + \boldsymbol{C}(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}) \tag{4.14}$$

with $\mathbb{A}$ a fourth-order and $\boldsymbol{C}$ a second-order constitutive tensor. Introducing (4.14) into the balance law of microforces (4.13) leads to

$$-\partial_{\boldsymbol{D}} \widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) - \mathbb{A}(\mathbb{e}, \boldsymbol{D})\dot{\boldsymbol{D}} - \boldsymbol{C}(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}}) + \boldsymbol{G} = \boldsymbol{0}. \tag{4.15}$$

If the fourth-order tensor $\mathbb{A}(\mathbb{e}, \boldsymbol{D})$ is non-singular, then the damage evolution law for the anisotropy tensor $\boldsymbol{D}$ is obtained as

$$\dot{\boldsymbol{D}} = \mathbb{A}(\mathbb{e}, \boldsymbol{D})^{-1}(\boldsymbol{G} - \partial_{\boldsymbol{D}} \widehat{\Psi}(\mathbb{e}, \boldsymbol{D}) - \boldsymbol{C}(\mathbb{e}, \boldsymbol{D}, \dot{\mathbb{e}})). \tag{4.16}$$

As a result, for quasi-static and isothermal process, the anisotropic damage evolution is described by Eqs. (4.11)–(4.16), if $\nabla \boldsymbol{D}$ can be neglected. Appropriate simplifications of the constitutive functions can be obtained following the ideas outlined in Section 3.

Assuming furthermore that also ∇d can be neglected—in general an incorrect assumption in the case of damage localization—local theories of anisotropic damage are obtained. In the literature a local model of anisotropic damage was presented by Murakami and Kamiya (1997) using a scalar and a tensor variable.

5. Conclusions

A thermodynamically consistent micromechanical theory for the analysis of damage evolution in thermo-viscoelastic and quasi-brittle materials is presented. It can be considered as a framework for the modeling of weakly nonlocal and gradient, respectively, damage theories. The main features can be summarized as follows.

- To describe isotropic and anisotropic damage, kinematical damage variables of scalar-, vector- and tensor-type are introduced.
- The theory is based on balance laws of macro- and microforces and first and second law of thermodynamics formulated for macro- and mesolevel.
- Inertia and kinetic energy of evolving microdefects and chemical reactions breaking internal material bonds are taken into account.
- General constitutive equations are formulated. From the Clausius–Duhem inequality it follows that the macro- and microforces consist of non-dissipative and dissipative parts. The dissipative microforces can be considered as driving forces on microdefects causing their motion.
- For isotropic damage the constitutive equations for various classes of material properties and process data are discussed in detail.
- For anisotropic damage described by a scalar and a tensor function, simplified gradient theories can be obtained, if the gradient of the anisotropy tensor can be neglected.

Further research work should be devoted to the determination of the constitutive functions for specified classes of material properties and process data and to the implementation of FE solution algorithms for gradient damage models.

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