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Thermodynamically based concept for the modelling of continua with microstructure and evolving defects

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Abstract

The aim of the paper is to present a thermodynamically based concept for the analysis of defect evolution in continua with microstructure. In classical models of continua with microstructure, balance laws for linear and angular momentum are formulated for macroforces and microforces, which can be called deformational macroforces and microforces. Characteristic feature of macrodefects and microdefects such as cracks and voids is the fact, that they can migrate relative to the moving body and this relative motion of defects is caused by so-called configurational forces. Therefore, in a continuum with microstructure and evolving macrodefects and microdefects we have to deal with deformational and configurational macroforces and microforces.

To formulate a reliable theory for material bodies with microstructure and migrating macrodefects and microdefects, a continuum is considered, where each particle is equipped with an arbitrary number of deformable directors. We distinguish then between directors undergoing a convective deformation leading to deformational (physical) microforces, and directors describing a set of defects migrating relative to the underlying lattice, where this migration is caused by configurational (material) microforces. For deformational and configurational macroforces and microforces corresponding balance laws are presented and the macro- and micro-Eshelby stress tensors are derived.

Next, deformational and configurational heatings and entropy fluxes are introduced and the first and second law of thermodynamics for the microcontinuum with evolving macrodefects and microdefects are formulated.

Finally, we present the most general form of the first order constitutive equations satisfying the second law of thermodynamics for migrating defects. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Continua with microstructure; Evolving defects; Configurational forces

1. Introduction

In lifetime oriented design of engineering structures a crucial role plays the analysis of defects together with a determination of the “driving” forces governing their evolution in the material. The term defect is used here to describe the observed departure from uniformity and inhomogeneity of the material on various

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scales. For example, on a microscale, there are point defects and dislocations in a crystal lattice, there can be shearbands, voids and cracks on a microlevel, and on the macrolevel shearbands, cavities and cracks can be observed. Here, we have to mention also phase boundaries separating martensite regions from their austenite twins and vice versa. Defects on various scales can alter their configuration and evolve through the material. Dislocations can glide and climb, point defects diffuse, cavities can change their shape, voids and cracks can evolve more or less independent of the motion of the surrounding mass, and interfaces can migrate. However, the motion of defects is entirely different from the motion of material bodies and sub-bodies in the physical space. Also the forces causing the evolution of defects are different from forces, which arise in response to motion and deformation of bodies in the physical space and which therefore can be called “deformational forces”. Since the forces on defects are associated with configurational changes in the structure of material bodies causing these changes, they are called “configurational forces”.

The fundamental concept of forces acting on defects in the material has its origin in the paper of Peach and Koehler (1950) on dislocations in crystalline material and the papers of Eshelby (1951, 1970) devoted to cracks and inclusions in linear elastic material.

During the last couple of years configurational forces on macrodefects attracted increasing interest with the aim to develop appropriate fracture and damage theories for the analysis of engineering structures. For example, the configurational force on a singular moving crack was investigated in Stumpf and Le (1990, 1992), Maugin and Trimarco (1992) and Maugin (1993, 1995), where further references can be found. In these papers forces associated with defects were derived as derivatives of the energy of the body with respect to certain tensors characterizing configurational changes of defects.

An approach to determine configurational forces on macrodefects, in some sense complementary to the above mentioned kinematical approach, was developed by Gurtin (1994, 1995) (see also Gurtin and Podio-Guidugli, 1992, 1996). In this concept configurational forces are regarded as primitive variables acting on so-called test regions, that can move independently of the motion of the body, where the configurational forces have to satisfy their own law of balance. Gurtin's considerations are based on the classical concept of continuous bodies in the sense of Cauchy, where the continuum exists of point-like particles having mass, inertia and supporting body and contact forces, but no internal structure. The concept of Gurtin was successfully applied by Fried and Gurtin (1996) and Cermelli and Fried (1997) to determine the motion of the interface in two-face materials.

More general continuous bodies, whose material particles may have an orientation and which are able to sustain couples and higher order forces, were extensively studied in the past with an attempt to provide an improved description of real properties of materials. Various theories of this kind are discussed in the literature, e.g. Toupin (1964), Ariman et al. (1973), Beatty and Cheverton (1976), Capriz and Podio-Guidugli (1977). More recently, Naghdi and Srinivasa (1993, 1994) and Le and Stumpf (1996a,b,c) presented nonlinear dislocation theories and models of finite elastoplasticity with microstructure, where the latter is based on the assumption of the multiplicative decomposition of the total deformation gradient into elastic and plastic parts first introduced by Bilby et al. (1955) and Kröner (1960).

Configurational forces and their balance in the presence of continua with microstructure are investigated in Maugin (1997, 1998) for an inhomogeneous–heterogeneous system and for polar elasticity, and in Stumpf and Saczuk (2000) for a dissipative oriented continuum using a variational approach with six-dimensional kinematics and manifold structure as point of departure.

Following the idea of Gurtin, who introduced the concept of configurational macroforces as primitive variables satisfying their own balance law, we present in this paper a thermodynamically based framework for the modelling of continua with microstructure and evolving macrodefects and microdefects. It is shown that one is led to configurational macroforces and microforces, which have to satisfy their own configurational macrobalance and microbalance laws. Taking into account that evolving defects have inertia and that they are dissipative, we generalize the classical first and second law of thermodynamics by taking into account the contributions of evolving macrodefects and microdefects.

In Section 2 continuous bodies with microstructure are considered. Following Ericksen and Truesdell (1958), each particle of the continuum is equipped with a finite number of vectors. The complete set of balance laws of mass, macromomentum, micromomentum, macroangular momentum and, within a thermodynamical theory, the balance law of energy and the principle of irreversibility are derived. Using the standard procedure of localization the corresponding dynamic field equations and the local form of the energy balance and of the irreversibility condition are obtained.

For continua with microstructure and macrodefects and microdefects Gurtin's concept of evolving test region is applied in Section 3 to derive configurational macroforces and microforces and effective forces. These forces are characterized by a suitable form of the mechanical power formulated for an arbitrary evolving test region.

In Section 4, the intrinsic configurational (inhomogeneity) forces and configurational momenta are introduced and the balance laws for configurational forces are formulated. Next, assuming that the total mechanical power for an evolving test region must be invariant with respect to the reparametrization of the bounding surface the general form of the Eshelby tensor for continua with microstructure and evolving defects is derived. In Section 5 the first and second law of thermodynamics are formulated taking into account macro- and micro-heatings and the associated entropy fluxes of deformational and configurational type.

In Section 6, the general form of the first order constitutive equations consistent with the previously derived laws of mechanics and thermodynamics is presented.

Finally, we want to point out that the investigations of this paper should be continued in two directions, where a restriction to continua with special microstructure seems to be meaningful (e.g. Cosserat continua, continua with three deformable directors that can be interpreted as orientation of the crystal lattice):

- (i) To take into account also distinguished cracks on singular surfaces (lines in the two-dimensional case) and to compare the results with those discussed in the literature (e.g. Freund, 1990; Hertzberg, 1996; Le et al., 1999).
- (ii) To use the general model of structured continua with evolving macrodefects and microdefects presented in this paper in order to derive corresponding phenomenological damage concepts for elastic and elastic–plastic material behavior and to compare them with well-established models in the literature (e.g. Gurson, 1977; Krajcinovic and Fonseka, 1981; Kachanov, 1986; Simo and Ju, 1987; Chaboche, 1988a,b; Krajcinovic, 1989; Hansen and Schreyer, 1994; Lubarda et al., 1994; Lubarda and Krajcinovic, 1995) by assuming the existence of damage and/or plastic potentials.

2. Thermodynamics of continua with microstructure

In this section we recall the basic laws of thermodynamics for various models of continua with microstructure. The notation and convention used subsequently are essentially standard, and hence they will be not discussed in details here (see e.g. Green and Naghdi, 1995).

In the simplest geometric description, a material body \mathcal{B} is defined as a continuum consisting of point-like particles, which at each time instant are continuously distributed over a region of space \mathcal{E} (the three-dimensional Euclidean space, whose translation space is denoted by E). Such regions are called spatial configurations of the body. For analytical purposes it is convenient to fix a particular configuration $B \subset \mathcal{E}$, called the reference configuration of the body, and to describe its motion and deformation with respect to this configuration. Then, $\mathbf{X} \in B$ is a place occupied by a generic particle $X \in \mathcal{B}$ in the reference configuration, and the macroscopic motion of the body relative to B is described by a mapping

$$\chi : B \times \mathcal{T} \rightarrow \mathcal{E}, \quad (\mathbf{X}, t) \rightarrow \mathbf{x} = \chi(\mathbf{X}, t) \quad (2.1)$$

which carries each point $\mathbf{X} \in B$ into its spatial place $\mathbf{x} \in B(t)$ in the actual configuration $B(t) = \chi(B, t)$ at time instant $t \in \mathcal{T}$.

Various generalizations of this model have been proposed in the literature by equipping each material particle with additional structure. Most of these generalizations can be regarded as special cases of the model first proposed by Ericksen and Truesdell (1957). This model consists of the classical concept of the body \mathcal{B} , each particle of which is additionally equipped with a finite number N of vectors, called directors. In the reference configuration, the directors assigned to a place $\mathbf{X} \in B$ are denoted by $\mathbf{d}_A(\mathbf{X})$, $A = 1, 2, \dots, N$. In general, there may be any number of vectors, even an infinite countable number.

Since the model of material body with microstructure is richer than the classical one, the description of motion consists of two parts. The directors in the current configuration assigned to every place $\mathbf{x} \in B(t)$ are denoted by $\bar{\mathbf{d}}_A(\mathbf{x}, t)$. Since $\mathbf{x} = \chi(\mathbf{X}, t)$, we may write in the referential description

$$\mathbf{d}_A(\mathbf{X}, t) = \bar{\mathbf{d}}_A(\chi(\mathbf{X}, t), t), \quad A = 1, 2, \dots, N. \quad (2.2)$$

The directors may change their length and orientation during the motion of the body through the physical space but they are carried by the material particles to which they are assigned.

The macrovelocity field $\mathbf{v}(\mathbf{X}, t)$ and the microvelocity fields $\mathbf{w}_A(\mathbf{X}, t)$ (the director velocities, as they are often called in the literature) are defined by

$$\mathbf{v}(\mathbf{X}, t) = \dot{\mathbf{x}}(\mathbf{X}, t), \quad \mathbf{w}_A(\mathbf{X}, t) = \dot{\mathbf{d}}_A(\mathbf{X}, t), \quad A = 1, 2, \dots, N. \quad (2.3)$$

Moreover, the macro- and the director deformation gradients are given by

$$\mathbf{F}(\mathbf{X}, t) = \nabla \chi(\mathbf{X}, t), \quad \mathbf{F}_A(\mathbf{X}, t) = \nabla \mathbf{d}_A(\mathbf{X}, t), \quad A = 1, 2, \dots, N. \quad (2.4)$$

If no special restrictions are imposed on the directors and their motion, the model of the continuous material body characterized in this way is commonly called Cosserat continuum with N deformable directors.

The physical meaning, which can be associated with the microstructure described by any number of deformable directors, will depend on the intended application of the theory. In general, the macromotion and micromotion are to some extent independent of each other. Accordingly, the classical balance laws of continuum mechanics do not suffice and they must be modified and enlarged by additional postulates.

Local theories of continuum mechanics are further based on the assumption that all physical properties of the material body can be represented as fields, and that the laws of motion are valid for every part of the body regardless of its size. In this context, a part of a body $\mathcal{P} \subset \mathcal{B}$, called sub-body, is understood as consisting always of the same material particles. Such a sub-body moves together with the body. In the reference configuration, the sub-body \mathcal{P} occupies a fixed sub-region $P \subset B$ having a time independent boundary ∂P . In the current configuration, it occupies the region $P(t) \subset B(t)$, which is the image of P under the deformation mapping, i.e. $P(t) = \chi(P, t)$ at every time instant $t \in \mathcal{T}$.

Early formulations of continua with microstructure were essentially based on variational arguments as in Toupin's (1964) theory of oriented hyperelastic materials or in the theory of liquid crystals by Ericksen (1961). Subsequently, their approach was refined and the basic laws of mechanics and thermodynamics valid for all material bodies were formulated and separated from the specific constitutive equations that define particular classes of materials (see e.g. Ericksen and Truesdell, 1958; Gurtin and Podio-Guidugli, 1992; Green and Naghdi, 1995). In the general case of a material body with any number of directors, the complete set of physical balance laws consists of (e.g. Green and Naghdi, 1995):

Balance of mass

$$\frac{d}{dt} \int_P \rho dv = 0, \quad (2.5)$$

Balance of macro-linear momentum

$$\frac{d}{dt} \int_P \mathbf{p} dv = \int_P \mathbf{f} dv + \int_{\partial P} \mathbf{T} \mathbf{n} da, \quad (2.6)$$

Balance of micro-linear momentum ($A = 1, 2, \dots, N$)

$$\frac{d}{dt} \int_P \mathbf{p}^A dv = \int_P (-\mathbf{k}^A + \mathbf{f}^A) dv + \int_{\partial P} \mathbf{T}^A \mathbf{n} da. \quad (2.7)$$

The balance law of macromomentum (2.6) has the same form as in the classical theory of continuum mechanics with all dynamic variables having their standard meaning: $\mathbf{p}(\mathbf{X}, t)$ is the referential macromomentum density, $\mathbf{f}(\mathbf{X}, t)$ is the external body force and $\mathbf{T}(\mathbf{X}, t)$ denotes the first Piola–Kirchhoff stress tensor. The balance law of macromomentum preserves its form in every theory of generalized continua. Truly new aspects of the theory are the additional balance laws of micromomentum (2.7). The new mechanical variables appearing in Eq. (2.7), not existing in the classical theories, are commonly named as follows:

- $\mathbf{p}^A(\mathbf{X}, t)$ – micromomenta,
- $\mathbf{f}^A(\mathbf{X}, t)$ – external microbody forces,
- $\mathbf{k}^A(\mathbf{X}, t)$ – intrinsic microbody forces,
- $\mathbf{T}^A(\mathbf{X}, t)$ – microstress tensors (of first Piola–Kirchhoff type).

The balance laws (2.5)–(2.7) must be supplemented by a suitable form of the balance of macro-angular momentum, where two classes of theories have to be distinguished. In the first class of theories it is assumed that microforces do not contribute to the balance of angular momentum, in which case this law takes the classical form

$$\frac{d}{dt} \int_P \mathbf{x} \times \mathbf{p} dv = \int_P \mathbf{x} \times \mathbf{f} dv + \int_{\partial P} \mathbf{x} \times \mathbf{T} \mathbf{n} da. \quad (2.8)$$

The other class of theories is based on the assumption that there is a coupling between microforces and macroforces, in which case the balance law (2.8) has to be replaced by

$$\frac{d}{dt} \int_P (\mathbf{x} \times \mathbf{p} + \mathbf{d}_A \times \mathbf{p}^A) dv = \int_P (\mathbf{x} \times \mathbf{f} + \mathbf{d}_A \times \mathbf{f}^A) dv + \int_{\partial P} (\mathbf{x} \times \mathbf{T} \mathbf{n} + \mathbf{d}_A \times \mathbf{T}^A \mathbf{n}) da. \quad (2.9)$$

In Eq. (2.9) and throughout the paper, the summation convention is applied to the diagonally repeated indices $A, B = 1, 2, \dots, N$.

The macro- and micro-momenta are assumed in the form

$$\mathbf{p} = \rho \mathbf{v}, \quad \mathbf{p}^A = \rho \alpha^{AB} \mathbf{w}_B, \quad (2.10)$$

where $\rho(\mathbf{X})$ is the referential mass density, and $\alpha^{AB}(\mathbf{X})$ are the microinertia coefficients, which are assumed to be time independent and to satisfy the following symmetry conditions: $\alpha^{AB} = \alpha^{BA}$ for all $A, B = 1, 2, \dots, N$.

Within purely mechanical theories, the balance laws (2.5)–(2.7) and (2.8) or (2.9) constitute the complete set of postulates, which are needed to determine the mechanical behavior of the material body with N deformable directors. Within thermodynamical theories, the body is further assumed to be equipped with thermal properties consistent with the balance law of energy and the principle of irreversibility. The balance law of energy is assumed in the form

$$\frac{d}{dt} \left\{ \int_P \rho \varepsilon dv + K(\mathcal{P}, t) \right\} = P(\mathcal{P}, t) + \int_P \rho r dv - \int_{\partial P} \mathbf{q} \cdot \mathbf{n} da, \quad (2.11)$$

where $K(\mathcal{P}, t)$ and $P(\mathcal{P}, t)$ denote the kinetic energy and the mechanical power, respectively. Moreover, $\varepsilon(\mathbf{X}, t)$ is the specific internal energy (the internal energy measured per unit mass), $r(\mathbf{X}, t)$, the heat absorption and $\mathbf{q}(\mathbf{X}, t)$ denotes the heat flux vector.

If the macromomentum and the micromomenta are assumed in the form (2.10), then the kinetic energy is given by

$$K(\mathcal{P}, t) = \frac{1}{2} \int_P \rho(\mathbf{v} \cdot \mathbf{v} + \alpha^{AB} \mathbf{w}_A \cdot \mathbf{w}_B) dv. \quad (2.12)$$

In Eq. (2.11) the mechanical power is defined by

$$P(\mathcal{P}, t) = \int_P (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial P} (\mathbf{T} \mathbf{n} \cdot \mathbf{v} + \mathbf{T}^A \mathbf{n} \cdot \mathbf{w}_A) da. \quad (2.13)$$

While the form (2.11) of the energy balance is commonly accepted in the literature of continuum thermodynamics, there are some disagreements as the second law of thermodynamics is concerned. Although different forms of this law were proposed in the literature, they all can be written in the form

$$\frac{d}{dt} \int_P \rho \eta dv \geq \int_P \rho s dv - \int_{\partial P} \mathbf{j} \cdot \mathbf{n} da, \quad (2.14)$$

where $\eta(\mathbf{X}, t)$ denotes the specific entropy (measured per unit mass), while $s(\mathbf{X}, t)$ and $\mathbf{j}(\mathbf{X}, t)$ stand for the source and flux of entropy (measured per unit mass and unit area). There is no general agreement in the literature, however, what precise form $s(\mathbf{X}, t)$ and $\mathbf{j}(\mathbf{X}, t)$ should have. In general, they are taken in the form

$$s(\mathbf{X}, t) = \frac{r(\mathbf{X}, t)}{\theta(\mathbf{X}, t)}, \quad \mathbf{j}(\mathbf{X}, t) = \frac{\mathbf{q}(\mathbf{X}, t)}{\theta(\mathbf{X}, t)} \quad (2.15)$$

in which case the second law of thermodynamics (2.14) takes the form of the Clausius–Duhem inequality. The common ratio $\theta(\mathbf{X}, t)$ is the absolute temperature, which by additional assumption is strictly positive, i.e. $\theta(\mathbf{X}, t) > 0$.

If sufficient regularity assumptions are presumed, the local form of the thermomechanical balance laws can be obtained by standard procedure. By virtue of Eq. (2.5), the referential mass density is time independent, $\dot{\rho} = 0$, so that the balance law of mass is identically satisfied. The standard procedure of localization applied to the mechanical balance laws (2.6) and (2.7) yields the following dynamic field equations:

Equilibrium equation of macroforces

$$\operatorname{div} \mathbf{T} + \mathbf{f} = \dot{\mathbf{p}}, \quad (2.16)$$

Equilibrium equations of microforces

$$\operatorname{div} \mathbf{T}^A - \mathbf{k}^A + \mathbf{f}^A = \dot{\mathbf{p}}^A, \quad A = 1, 2, \dots, N. \quad (2.17)$$

If the balance law of angular momentum is taken in the form (2.8), then we obtain the equilibrium equation of macrocouples

$$\mathbf{T} \mathbf{F}^T - \mathbf{F} \mathbf{T}^T = 0 \quad (2.18)$$

which is just the assertion that the true (Cauchy) stress tensor must be symmetric. In the more general case, when the balance law of angular momentum is taken in the form (2.9) its local form reads

$$\mathbf{T} \mathbf{F}^T - \mathbf{F} \mathbf{T}^T + \mathbf{d}_A \wedge \mathbf{k}^A + \mathbf{T}^A \mathbf{F}_A^T - \mathbf{F}_A (\mathbf{T}^A)^T = 0. \quad (2.19)$$

Here $\mathbf{a} \wedge \mathbf{b} = \mathbf{a} \otimes \mathbf{b} - \mathbf{b} \otimes \mathbf{a}$ is the standard notation for the exterior product of any two vectors, and \otimes denotes the tensor product of two vectors.

The net working (the total power expanded) $W(\mathcal{P}, t)$ for every sub-body \mathcal{P} is defined by

$$W(\mathcal{P}, t) = P(\mathcal{P}, t) - \dot{K}(\mathcal{P}, t), \quad (2.20)$$

and, in view of Eqs. (2.12) and (2.13), is given by

$$W(\mathcal{P}, t) = \int_P \{(\mathbf{f} - \dot{\mathbf{p}}) \cdot \mathbf{v} + (\mathbf{f}^A - \dot{\mathbf{p}}^A) \cdot \mathbf{w}_A\} dv + \int_{\partial P} (\mathbf{T}\mathbf{n} \cdot \mathbf{v} + \mathbf{T}^A\mathbf{n} \cdot \mathbf{w}_A) da. \quad (2.21)$$

Moreover, under the assumption that the balance laws (2.6) and (2.7) hold, it can be shown that

$$W(\mathcal{P}, t) = \int_P \sigma dv, \quad \sigma = \mathbf{T} \cdot \dot{\mathbf{F}} - \mathbf{k}^A \cdot \mathbf{w}_A + \mathbf{T}^A \cdot \dot{\mathbf{F}}_A, \quad (2.22)$$

where $\sigma(\mathbf{X}, t)$ is the stress power density measured per unit volume of the reference configuration.

With the use of Eq. (2.20) the balance law of energy (2.11) can be rewritten in the form

$$\frac{d}{dt} \int_P \rho \varepsilon dv = W(\mathcal{P}, t) + \int_P \rho r dv - \int_{\partial P} \mathbf{q} \cdot \mathbf{n} da. \quad (2.23)$$

Then by virtue of Eq. (2.22), the local form of the energy balance is obtained as

$$\rho \dot{\varepsilon} = \sigma + \rho r - \operatorname{div} \mathbf{q}. \quad (2.24)$$

The principle of irreversibility (second law of thermodynamics) (2.14) together with the assumptions (2.15) yields

$$\rho \dot{\eta} \geq \rho \theta^{-1} r - \operatorname{div}(\theta^{-1} \mathbf{q}). \quad (2.25)$$

Introducing next the free energy function

$$\psi(\mathbf{X}, t) = \varepsilon(\mathbf{X}, t) - \theta(\mathbf{X}, t) \eta(\mathbf{X}, t), \quad (2.26)$$

the reduced dissipation inequality implied by Eq. (2.25) takes the form

$$\dot{\psi} + \dot{\theta} \eta - \sigma + \theta^{-1} \mathbf{q} \cdot \nabla \theta \leq 0. \quad (2.27)$$

The set of Eqs. (2.16)–(2.27) has to be completed by a suitable set of constitutive equations.

In most problems of continuum thermomechanics, the body force \mathbf{f} , the director body forces \mathbf{f}^A and the heat absorption r are specified as part of the data. Then, the first Piola–Kirchhoff macrostress tensor \mathbf{T} , the director stress vectors \mathbf{k}^A and the microstress tensors \mathbf{T}^A , the heat flux vector \mathbf{q} , the internal energy ε (or, equivalently, the free energy ψ) and the entropy η must be specified in terms of the history of macromotion χ and micromotion described by the directors \mathbf{d}_A and the temperature θ .

3. Evolving defects and configurational forces

In this section we want to investigate defects on the macrolevel and microlevel migrating relative to the moving body, where the defect evolution is caused by configurational macroforces and microforces. We will follow Gurtin (1994, 1995), who introduced the concept of an evolving nonmaterial test region to characterize configurational macroforces and evolving macrodefects.

In the reference configuration B of the body, an evolving test region is defined as a closed and simply connected subset $R(t) \subset B$, whose boundary surface $\partial R(t)$ evolves smoothly with time (Fig. 1). The test region should not be confused with a sub-body, that occupies in the reference configuration the fixed region $P \subset B$, representing a part of the body and having the time independent boundary ∂P . A test region is not a fixed part of the body, but can migrate through the reference configuration B of the body.

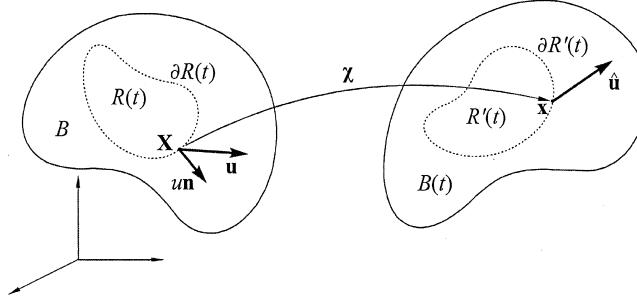


Fig. 1. Test region in the reference and actual configuration of the body.

For a test region $R(t)$, $\mathbf{n}(\mathbf{X}, t)$ will denote the outward normal to the boundary surface $\partial R(t)$, $\mathbf{u}(\mathbf{X}, t)$ the velocity of $\partial R(t)$ and $u(\mathbf{X}, t)$ its normal component, i.e. the velocity in the direction of $\mathbf{n}(\mathbf{X}, t)$

$$u(\mathbf{X}, t) = \mathbf{u}(\mathbf{X}, t) \cdot \mathbf{n}(\mathbf{X}, t). \quad (3.1)$$

When confusion can arise we write $\mathbf{n}_{\partial R(t)}(\mathbf{X}, t)$ for the outward normal to $\partial R(t)$, while keeping the notation $\mathbf{n}(\mathbf{X})$ for the outward normal to the boundary ∂P of any sub-body. If the boundary surface $\partial R(t)$ is described in the parametric form $\mathbf{X} = \mathbf{X}(\xi, t)$, where $\xi = (\xi^\alpha)$, $\alpha = 1, 2$, are surface coordinates, then the velocity of a generic point of $\partial R(t)$ is defined by

$$\mathbf{u}(\xi, t) = \frac{d}{dt} \mathbf{X}(\xi, t)_{|\xi=\text{const.}}. \quad (3.2)$$

However, the velocity $\mathbf{u}(\mathbf{X}, t)$ depends on the choice of the local parametrization of $\partial R(t)$, and only the normal component $u(\mathbf{X}, t)$ is parametrization independent. In the referential description, the motion of a body is described by a mapping $\mathbf{x} = \gamma(\mathbf{X}, t)$, and the current configuration of the body at time instant t is defined by $B(t) = \gamma(B, t)$. Then, for the evolving test region $R(t) \subset B$ we set $R'(t) = \gamma(\partial R(t), t)$. Moreover, for $\partial R(t)$ given in the parametric form $\mathbf{X} = \mathbf{X}(\xi, t)$, the boundary surface $\partial R'(t) \equiv \gamma(\partial R(t), t)$ of the test region evolving in the current configuration is described by

$$\mathbf{x}(\xi, t) = \gamma(\mathbf{X}(\xi, t), t), \quad (3.3)$$

and the induced velocity of a generic point at $\partial R'(t)$ is defined by

$$\hat{\mathbf{u}}(\xi, t) \equiv \frac{d}{dt} \mathbf{x}(\xi, t)_{|\xi=\text{const.}}. \quad (3.4)$$

From the chain rule applied to Eq. (3.4) we then have

$$\hat{\mathbf{u}}(\gamma(\mathbf{X}, t), t) = \mathbf{v}(\mathbf{X}, t) + \mathbf{F}(\mathbf{X}, t) \mathbf{u}(\mathbf{X}, t), \quad (3.5)$$

where the material velocity field $\mathbf{v}(\mathbf{X}, t)$ and the deformation gradient $\mathbf{F}(\mathbf{X}, t)$ of the moving body are defined in Eqs. (2.3) and (2.4), respectively.

The evolving test region $R(t) \subset B$ is regarded as a region containing continuously distributed defects in the body, and since the motion of the boundary $\partial R(t)$ in B represents a kinematical process independent of the motion of the material particles, the configurational forces can be introduced through the power expended on $\partial R(t)$. In other words, for $\partial R(t)$ to evolve smoothly with the velocity $\mathbf{u}(\mathbf{X}, t)$, there must exist a configurational stress field $\mathbb{C}(\mathbf{X}, t)$ that acts on $\partial R(t)$ and governs its evolution. Thus $R(t)$ may contain structural defects, and the configurational traction associated with $\mathbb{C}\mathbf{n}$ represents then the resultant of the total force exerted on these defects by that part of B external to $R(t)$. By definition, the configurational stresses expend power by the velocity $\mathbf{u}(\mathbf{X}, t)$ so that its working on $R(t)$ is

$$\int_{\partial R(t)} \mathbb{C}\mathbf{n} \cdot \mathbf{u} da. \quad (3.6)$$

For an evolving test region $R(t)$, the deformational traction \mathbf{Tn} should act on the velocity $\hat{\mathbf{u}}(\mathbf{x}, t)$. Hence, the working on $\partial R(t)$ of the deformational stress has the form

$$\int_{\partial R(t)} \mathbf{Tn} \cdot \hat{\mathbf{u}} da. \quad (3.7)$$

Besides the deformational surface force $\mathbf{t}_n = \mathbf{Tn}$ we have to take into account the external body force \mathbf{f} . Correspondingly, the system of configurational forces consists of the configurational surface force $\mathbb{C}_n = \mathbb{C}\mathbf{n}$ and the intrinsic configurational (inhomogeneity) force $\mathbb{f}(\mathbf{X}, t)$. However, unlike the external body force \mathbf{f} , the intrinsic configurational force \mathbb{f} does not contribute to the power expended on $R(t)$. Accordingly, in view of Eqs. (3.6) and (3.7) the power expended on $R(t)$ can be written as

$$P(R(t)) = \int_{R(t)} \mathbf{f} \cdot \mathbf{v} dv + \int_{\partial R(t)} (\mathbf{Tn} \cdot \hat{\mathbf{u}} + \mathbb{C}\mathbf{n} \cdot \mathbf{u}) da. \quad (3.8)$$

If the body has a microstructure described by N deformable directors associated with every material particle, the kinematics of an evolving test region is richer than in Gurtin's macrotheory. In fact, the directors $\mathbf{D}_A(\mathbf{X})$ associated with every material point $\mathbf{X} \in B$ are time independent. However, they become time dependent when considered at the boundary surface $\partial R(t)$ of the evolving test region $R(t) \subset B$. Assuming that $\partial R(t)$ is given in the parametric form $\mathbf{X} = \mathbf{X}(\xi, t)$, we have

$$\mathbf{D}_A(\xi, t) = \mathbf{D}_A(\mathbf{X}(\xi, t)), \quad A = 1, 2, \dots, N. \quad (3.9)$$

Denoting by $\mathbf{D}_A^\circ(\xi, t)$ the time derivative of $\mathbf{D}_A(\mathbf{X})$ while keeping $\xi = \text{const.}$ and making use of Eq. (3.2) we have

$$\mathbf{D}_A^\circ(\xi, t) = \nabla \mathbf{D}_A(\xi, t) \mathbf{X}^\circ(\xi, t) = \nabla \mathbf{D}_A(\xi, t) \mathbf{u}(\xi, t). \quad (3.10)$$

It follows that for the body with microstructure every point at the boundary of the evolving test region is characterized, aside of $\mathbf{u}(\mathbf{X}, t)$, by N velocity vectors

$$\mathbf{u}_A(\mathbf{X}, t) \equiv \mathbf{D}_A^\circ(\mathbf{X}, t) = \mathbf{G}_A(\mathbf{X}, t) \mathbf{u}(\mathbf{X}, t), \quad \mathbf{G}_A(\mathbf{X}, t) \equiv \nabla \mathbf{D}_A(\mathbf{X}, t). \quad (3.11)$$

It is further seen that these velocity vectors are entirely determined by $\mathbf{u}(\mathbf{X}, t)$ and the referential gradients \mathbf{G}_A of the directors. Thus $\mathbf{u}(\mathbf{X}, t)$ and \mathbf{G}_A define completely the evolution of the microstructure at the boundary $\partial R(t)$ of the evolving test region $R(t)$.

We next need to derive the evolution of the microstructure in the current configuration $B(t)$ of the body. To this end, the directors $\mathbf{d}_A(\mathbf{x}, t)$ in $B(t)$, when considered at the boundary surface $\partial R'(t) = \chi(\partial R(t), t)$ of the evolving test region, are written as

$$\mathbf{d}_A(\xi, t) = \mathbf{d}_A(\mathbf{x}(\xi, t), t), \quad (3.12)$$

where $\mathbf{x}(\xi, t)$ is defined by Eq. (3.3). The time derivative $\mathbf{d}_A^\circ(\xi, t)$ of Eq. (3.12) is obtained by using the chain rule as

$$\mathbf{d}_A^\circ = \partial_t \mathbf{d}_A + (\text{grad } \mathbf{d}_A) \hat{\mathbf{u}}. \quad (3.13)$$

Further, taking into account Eq. (3.5) we have

$$\mathbf{d}_A^\circ = \partial_t \mathbf{d}_A + (\text{grad } \mathbf{d}_A)(\mathbf{v} + \mathbf{F}\mathbf{u}) = \partial_t \mathbf{d}_A + (\text{grad } \mathbf{d}_A) \mathbf{v} + (\text{grad } \mathbf{d}_A) \mathbf{F}\mathbf{u}. \quad (3.14)$$

The material time derivative $\dot{\mathbf{d}}_A(\mathbf{y}, t)$ of the directors in the current configuration is defined by

$$\mathbf{w}_A \equiv \dot{\mathbf{d}}_A = \partial_t \mathbf{d}_A + (\text{grad } \mathbf{d}_A) \mathbf{v}, \quad (3.15)$$

and from the chain rule we have

$$\nabla \mathbf{d}_A = (\text{grad } \mathbf{d}_A) \mathbf{F}, \quad (3.16)$$

where $\mathbf{F}(\mathbf{X}, t)$ denotes the macrodeformation gradient. Substituting Eq. (3.15) into Eq. (3.13) and making use of Eq. (3.14) leads to

$$\hat{\mathbf{u}}_A \equiv \mathbf{d}_A^\circ = \dot{\mathbf{d}}_A + (\nabla \mathbf{d}_A) \mathbf{u} = \mathbf{w}_A + \mathbf{F}_A \mathbf{u}, \quad \mathbf{F}_A \equiv \nabla \mathbf{d}_A. \quad (3.17)$$

Thus the migration of the test region in the current configuration of the body is completely determined by the velocity vectors $\hat{\mathbf{u}}$ and $\hat{\mathbf{u}}_A$, $A = 1, 2, \dots, N$.

Within theories of continua with microstructure, the response of a body to motion and deformation is described by standard forces and director forces consistent with the fundamental laws of mechanics presented in Section 2. In order to introduce the concept of configurational forces for continua with microstructure, we first note that the boundary $\partial R(t)$ of the evolving test region is characterized by the velocity $\mathbf{u}(\mathbf{X}, t)$ and structural velocities $\mathbf{u}_A(\mathbf{X}, t)$, while for continua without microstructure only the velocity $\mathbf{u}(\mathbf{X}, t)$ exists. Thus, in the case of continua with microstructure, the working equation (3.6) must be replaced by the more general expression

$$\int_{\partial R(t)} (\mathbb{C} \mathbf{n} \cdot \mathbf{u} + \mathbb{C}^A \mathbf{n} \cdot \mathbf{u}_A) da, \quad (3.18)$$

which represents the working of the configurational macrostress tensor $\mathbb{C}(\mathbf{X}, t)$ and the configurational microstress tensors $\mathbb{C}^A(\mathbf{X}, t)$, $A = 1, 2, \dots, N$, at the boundary $\partial R(t)$.

Within continua with microstructure, the working of the deformational stresses and deformational director stresses on $\partial R(t)$ is given by (corresponding to the boundary term in the expression for the mechanical power (2.13))

$$\int_{\partial R(t)} (\mathbf{T} \mathbf{n} \cdot \hat{\mathbf{u}} + \mathbf{T}^A \mathbf{n} \cdot \hat{\mathbf{u}}_A) da. \quad (3.19)$$

Moreover, there are external body macroforce $\mathbf{f}(\mathbf{X}, t)$ and microforces $\mathbf{f}^A(\mathbf{X}, t)$, which must be taken into account when considering the mechanical power expended on $R(t)$. There will be also intrinsic configurational (inhomogeneity) macroforce $\mathbf{f}(\mathbf{X}, t)$ and intrinsic configurational microforces $\mathbf{f}^A(\mathbf{X}, t)$. However, like the intrinsic microforces $\mathbf{k}^A(\mathbf{X}, t)$, neither $\mathbf{f}(\mathbf{X}, t)$ nor $\mathbf{f}^A(\mathbf{X}, t)$ contribute to the power expended on $R(t)$, which is given by

$$\mathcal{P}(R(t)) = \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} (\mathbf{T} \mathbf{n} \cdot \hat{\mathbf{u}} + \mathbf{T}^A \mathbf{n} \cdot \hat{\mathbf{u}}_A + \mathbb{C} \mathbf{n} \cdot \mathbf{u} + \mathbb{C}^A \mathbf{n} \cdot \mathbf{u}_A) da. \quad (3.20)$$

Using Eqs. (3.5) and (3.17) we obtain

$$\mathcal{P}(R(t)) = \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} \{ \mathbf{T} \mathbf{n} \cdot (\mathbf{v} + \mathbf{F} \mathbf{u}) + \mathbf{T}^A \mathbf{n} \cdot (\mathbf{w}_A + \mathbf{F}_A \mathbf{u}) + \mathbb{C} \mathbf{n} \cdot \mathbf{u} + \mathbb{C}^A \mathbf{n} \cdot \mathbf{G}_A \mathbf{u} \} da. \quad (3.21)$$

We can rewrite Eq. (3.21) in the form

$$\mathcal{P}(R(t)) = \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} \{ \mathbf{T} \mathbf{n} \cdot \mathbf{v} + \mathbf{T}^A \mathbf{n} \cdot \mathbf{w}_A + (\mathbf{F}^T \mathbf{T} + \mathbb{C} + \mathbf{F}_A^T \mathbf{T}^A + \mathbf{G}_A^T \mathbb{C}^A) \mathbf{n} \cdot \mathbf{u} \} da. \quad (3.22)$$

In the case of continua without microstructure, we have $\mathbf{w}_A = \mathbf{0}$, $\mathbf{G}_A = \mathbf{F}_A = \mathbf{0}$, and the mechanical power (3.22) reduces to the form presented by Gurtin (1995). For a stationary test region, $\mathbf{u} = \mathbf{0}$, expression (3.22) leads to the classical form of the expended power of contact forces (2.13).

4. Configurational inertia and balance laws of configurational forces

In Gurtin's approach configurational forces are viewed as basic primitive objects which must be consistent with their own law of balance. Cermelli and Fried (1997) noted furthermore that although evolving defects have no mass, they have their own inertia. In an effort to account properly for configurational inertia, they slightly modified Gurtin's approach by assuming that besides the configurational stress tensor $\mathbb{C}(\mathbf{X}, t)$ and the intrinsic configurational force $\mathbf{f}(\mathbf{X}, t)$, there should exist a configurational momentum $\mathbf{p}(\mathbf{X}, t)$. Then, for continua without microstructure, they postulated the following local form of the configurational balance law:

$$\operatorname{div} \mathbb{C} + \mathbf{f} = \dot{\mathbf{p}}. \quad (4.1)$$

In this section we shall generalize Gurtin's and Cermelli and Fried's approach for continua with arbitrary microstructure.

To describe problems where the microstructure of the body can undergo configurational changes due to microdefects migrating relative to the underlying lattice, we have introduced in the previous section the configurational microstress tensors $\mathbb{C}^A(\mathbf{X}, t)$ and configurational intrinsic forces $\mathbf{f}^A(\mathbf{X}, t)$. To account for the inertia of evolving defects in the body with microstructure we further assume that, besides the configurational macromomentum $\mathbf{p}(\mathbf{X}, t)$, there should exist configurational micromomenta $\mathbf{p}^A(\mathbf{X}, t)$, $A = 1, 2, \dots, N$. Taking into account that deformational and configurational balance laws can be derived by variation of a Lagrangian functional formulated within a materio-physical manifold (see e.g. Stumpf and Saczuk, 2000), we postulate the following form of the microbalance law:

$$\operatorname{div} \mathbb{C}^A + \mathbf{f}^A = \dot{\mathbf{p}}^A, \quad A = 1, 2, \dots, N. \quad (4.2)$$

The configurational balance laws, which merely assert that the total configurational force be balanced over each part of the body, are supplemental laws to be imposed in addition to the standard balance laws of the classical theory, with the understanding that they degenerate to an identity (in fact, equivalent to the linear momentum balance) in the absence of configurational changes of the body.

By virtue of the transport theorem for the evolving test region

$$\frac{d}{dt} \int_{R(t)} \psi dv = \int_{R(t)} \dot{\psi} dv + \int_{\partial R(t)} u \psi da = \int_{R(t)} \dot{\psi} dv + \int_{\partial R(t)} (\psi \otimes \mathbf{u}) \mathbf{n} da \quad (4.3)$$

for any field $\psi(\mathbf{X}, t)$, where $u = \mathbf{u} \cdot \mathbf{n}$ denotes the normal velocity of the boundary surface $\partial R(t)$, the configurational balance laws (4.1) and (4.2) for every test region $R(t)$ migrating in the reference configuration of the body are equivalent to the following postulates:

$$\begin{aligned} \int_{R(t)} \mathbf{f} dv + \int_{\partial R(t)} (\mathbb{C} + \mathbf{p} \otimes \mathbf{u}) \mathbf{n} da &= \frac{d}{dt} \int_{R(t)} \mathbf{p} dv, \\ \int_{R(t)} \mathbf{f}^A dv + \int_{\partial R(t)} (\mathbb{C}^A + \mathbf{p}^A \otimes \mathbf{u}) \mathbf{n} da &= \frac{d}{dt} \int_{R(t)} \mathbf{p}^A dv. \end{aligned} \quad (4.4)$$

Accordingly, the total mechanical power exerted on the test region $R(t)$ is given by

$$\begin{aligned} W(R(t)) &= \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} \{(\mathbf{T} + \mathbf{p} \otimes \mathbf{u}) \mathbf{n} \cdot \hat{\mathbf{u}} + (\mathbf{T}^A + \mathbf{p}^A \otimes \mathbf{u}) \mathbf{n} \cdot \hat{\mathbf{u}}_A\} da \\ &\quad + \int_{\partial R(t)} \{(\mathbb{C} + \mathbf{p} \otimes \mathbf{u}) \mathbf{n} \cdot \mathbf{u} + (\mathbb{C}^A + \mathbf{p}^A \otimes \mathbf{u}) \mathbf{n} \cdot \mathbf{u}_A\} da. \end{aligned} \quad (4.5)$$

Taking into account that the fields $\hat{\mathbf{u}}$ and $\hat{\mathbf{u}}_A$ are defined by Eqs. (3.5) and (3.17), respectively, the total mechanical power (4.5) can be rewritten in the form

$$W(R(t)) = \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} \{(\mathbf{T} + \mathbf{p} \otimes \mathbf{u}) \mathbf{n} \cdot \mathbf{v} + (\mathbf{T}^A + \mathbf{p}^A \otimes \mathbf{u}) \mathbf{n} \cdot \mathbf{w}_A + (\mathbf{Hn} + u\mathbf{h}) \cdot \mathbf{u}\} da, \quad (4.6)$$

where the tensor $\mathbf{H}(\mathbf{X}, t)$ and the vector $\mathbf{h}(\mathbf{X}, t)$ are defined by

$$\begin{aligned} \mathbf{H} &\equiv \mathbf{F}^T \mathbf{T} + \mathbf{F}_A^T \mathbf{T}^A + \mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A, \\ \mathbf{h} &\equiv \mathbf{F}^T \mathbf{p} + \mathbf{F}_A^T \mathbf{p}^A + \mathbb{p} + \mathbf{F}_A^T \mathbb{p}^A. \end{aligned} \quad (4.7)$$

For the evolving test region there is no intrinsic material description of its boundary $\partial R(t)$. Changes in parametrization of $\partial R(t)$ affect the tangential component of its evolution velocity $\mathbf{u}(\mathbf{x}, t)$, but leaves its normal component $u(\mathbf{x}, t)$ unaltered. In effect, invariance of the total mechanical power (4.6) under the change of reparametrization of $\partial R(t)$ is equivalent to the requirement that

$$(\mathbf{Hn} + u\mathbf{h}) \cdot \boldsymbol{\tau} = 0 \quad (4.8)$$

on $\partial R(t)$ for all tangential vector fields $\boldsymbol{\tau}$ along the evolving boundary $\partial R(t)$. Thus the expression $(\mathbf{Hn} + u\mathbf{h})$ must be parallel to the normal vector \mathbf{n} of $\partial R(t)$, and since it is arbitrary, we obtain

$$\mathbf{Hn} + u\mathbf{h} = \pi\mathbf{n}, \quad (4.9)$$

where the scalar field $\pi(\mathbf{x}, t)$ can be considered as configurational tension. By virtue of Eq. (4.9) the total power (4.6) expended on $R(t)$ is given by the expression

$$W(R(t)) = \int_{R(t)} (\mathbf{f} \cdot \mathbf{v} + \mathbf{f}^A \cdot \mathbf{w}_A) dv + \int_{\partial R(t)} \{ \mathbf{Tn} \cdot \mathbf{v} + \mathbf{T}^A \mathbf{n} \cdot \mathbf{w}_A + u(\mathbf{p} \cdot \mathbf{v} + \mathbf{p}^A \cdot \mathbf{w}_A + \pi) \} da \quad (4.10)$$

which is invariant with respect to the reparametrization of $\partial R(t)$. Moreover, the identity (4.9) must hold for all test regions $R(t)$ with an evolution of their boundaries $\partial R(t)$ being completely determined by the normal vector \mathbf{n} and the normal velocity u . In other words, Eq. (4.8) must hold for any choice of \mathbf{n} and u . This implies that \mathbf{h} is proportional to \mathbf{n} for any \mathbf{n} . Thus we have

$$\mathbf{h} \equiv \mathbf{F}^T \mathbf{p} + \mathbf{F}_A^T \mathbf{p}^A + \mathbb{p} + \mathbf{G}_A^T \mathbb{p}^A = \mathbf{0}, \quad (4.11)$$

and consequently

$$\mathbf{Hn} = \pi\mathbf{n}. \quad (4.12)$$

From Eq. (4.11) it follows that the configurational momenta \mathbb{p} and \mathbb{p}^A are determined by the relation

$$\mathbb{p} + \mathbf{G}_A^T \mathbb{p}^A = -(\mathbf{F}^T \mathbf{p} + \mathbf{F}_A^T \mathbf{p}^A), \quad (4.13)$$

and from Eq. (4.12) follows that the configurational stress tensors are given by

$$\mathbf{F}^T \mathbf{T} + \mathbf{F}_A^T \mathbf{T}^A + \mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A = \pi \mathbf{1}, \quad (4.14)$$

where $\mathbf{1}$ denotes the unit tensor.

The physical meaning of the configurational tension $\pi(\mathbf{x}, t)$ can be observed using the second law of thermodynamics, which reduces within a purely mechanical theory to

$$\frac{d}{dt} \int_{R(t)} \rho \psi dv \leq W(R(t)). \quad (4.15)$$

By virtue of the transport theorem (4.3), the inequality (4.15) can be rewritten in the form

$$\int_{R(t)} \rho \psi dv \leq W(R(t)) - \int_{\partial R(t)} \rho \psi \mathbf{n} \cdot \mathbf{u} da. \quad (4.16)$$

Having in mind that the total mechanical power is given by Eq. (4.10) the requirement of invariance of (4.16) with respect to the reparametrization implies that the configurational tension $\pi(\mathbf{X}, t)$ is given by

$$\pi = \rho\psi - \frac{1}{2}\rho(\mathbf{v} \cdot \mathbf{v} + \alpha^{AB}\mathbf{w}_A \cdot \mathbf{w}_B). \quad (4.17)$$

Substituting now Eq. (4.17) into Eq. (4.14) we finally obtain

$$\mathbf{F}^T \mathbf{T} + \mathbf{F}_A^T \mathbf{T}^A + \mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A = \{\Psi - \frac{1}{2}\rho(\mathbf{v} \cdot \mathbf{v} + \alpha^{AB}\mathbf{w}_A \cdot \mathbf{w}_B)\} \mathbf{1}, \quad (4.18)$$

where $\Psi \equiv \rho\psi$ denotes the free energy function measured per unit volume of the reference configuration of the body. The relation (4.18), which can be rewritten in the form

$$\mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A = \{\Psi - \frac{1}{2}\rho(\mathbf{v} \cdot \mathbf{v} + \alpha^{AB}\mathbf{w}_A \cdot \mathbf{w}_B)\} \mathbf{1} - (\mathbf{F}^T \mathbf{T} + \mathbf{F}_A^T \mathbf{T}^A), \quad (4.19)$$

yields a generalization of the classical Eshelby relation. Indeed, as special case of a continuum without microstructure we have

$$\mathbb{C} = (\Psi - \frac{1}{2}\rho\mathbf{v} \cdot \mathbf{v}) \mathbf{1} - \mathbf{F}^T \mathbf{T} \quad (4.20)$$

leading in the quasi-static case to

$$\mathbb{C} = \Psi \mathbf{1} - \mathbf{F}^T \mathbf{T} \quad (4.21)$$

representing the classical Eshelby tensor. It is important to note here that the generalized Eshelby relation (4.19) and the special cases (4.20) and (4.21) were derived without recourse to special constitutive assumptions. They are valid for dissipative and nondissipative processes.

5. Configurational heating and laws of thermodynamics

Within a purely mechanical theory structural changes in a material body due to evolving defects are determined by the configurational stresses, forces and momenta as discussed in detail in the previous section. However, such structural changes in the material body are in general dissipative and therefore any theory of continua with evolving defects should be based on the thermodynamics of irreversible processes. It is then necessary to supplement our equations derived in the previous sections by formulating appropriate forms of the first and second laws of thermodynamics, the balance law of energy and the principle of irreversibility. For continua with microstructure, but without migration of defects, these two laws of thermodynamics are given by Eqs. (2.11) and (2.14), respectively.

Within the context of classical continua (continua without microstructure), the laws of thermodynamics in the presence of evolving defects were considered by Fried and Gurtin (1996). They introduced the configurational heating $Q(\mathbf{X}, t)$ and the associated configurational entropy flux $\mathbf{j}(\mathbf{X}, t)$ assumed in the form $\mathbf{j} = \theta^{-1}Q\mathbf{n}$, which are defined by

$$\int_{\partial R(t)} Q\mathbf{n} \cdot \mathbf{u} da, \quad \int_{\partial R(t)} (\theta^{-1}Q\mathbf{n}) \cdot \mathbf{u} da, \quad (5.1)$$

respectively. Here $\theta(\mathbf{X}, t)$ denotes the absolute temperature, and $\mathbf{u}(\mathbf{X}, t)$ is the velocity of $\partial R(t)$ defined by Eq. (3.2). Using these fields Fried and Gurtin (1996) formulated the balance of energy and the principle of irreversibility for an arbitrary control region $R(t)$ evolving in the reference configuration of the body.

In the case of continua with microstructure the configurational heating should be of two kinds, the configurational heating $Q(\mathbf{X}, t)$ resulting from the interactions of the evolving defects with the bulk material of the body and the configurational microheatings $Q^A(\mathbf{X}, t)$, $A = 1, 2, \dots, N$, resulting from the interactions of the evolving defects with the fine structure of the material body, which is described by N directors. These configurational heatings are characterized by

$$\int_{\partial R(t)} (Q\mathbf{n} \cdot \mathbf{u} + Q^A \mathbf{n} \cdot \mathbf{u}_A) da. \quad (5.2)$$

Accordingly, the law of energy balance (2.11) rewritten for the evolving test region $R(t)$ taking into account Eq. (5.2) reads

$$\frac{d}{dt} \left\{ \int_{R(t)} \rho \varepsilon dv + K(R(t)) \right\} = P(R(t)) + \int_{R(t)} \rho r dv - \int_{\partial R(t)} (\mathbf{q} \cdot \mathbf{n} + Q\mathbf{n} \cdot \mathbf{u} + Q^A \mathbf{n} \cdot \mathbf{u}_A) da \quad (5.3)$$

with the kinetic energy $K(R(t))$ and the total mechanical power $W(R(t))$ of the evolving test region given by Eqs. (2.12) and (4.10), respectively.

In consistency with Eq. (5.2) we next assume the configurational macro- and micro-entropy fluxes in the form $\mathbf{j} = \theta^{-1} Q\mathbf{n}$ and $\mathbf{j}^A = \theta^{-1} Q^A \mathbf{n}$, $A = 1, 2, \dots, N$, leading to the total configurational entropy flux

$$\int_{\partial R(t)} \{(\theta^{-1} Q\mathbf{n}) \cdot \mathbf{u} + (\theta^{-1} Q^A \mathbf{n}) \cdot \mathbf{u}_A\} da. \quad (5.4)$$

With Eq. (5.4) the principle of irreversibility (2.14) rewritten for the evolving test region takes the form

$$\frac{d}{dt} \int_{R(t)} \rho \eta dv \geq \int_{R(t)} \rho \theta^{-1} r dv - \int_{\partial R(t)} \{(\theta^{-1} \mathbf{q}) \cdot \mathbf{n} + (\theta^{-1} Q\mathbf{n}) \cdot \mathbf{u} + (\theta^{-1} Q^A \mathbf{n}) \cdot \mathbf{u}_A\} da \quad (5.5)$$

provided that the assumption (2.15) holds.

Both principles of thermodynamics must be invariant with respect to the reparametrization of the boundary $\partial R(t)$ of the evolving test region. Keeping in mind that $\mathbf{u}_A = \mathbf{G}_A \mathbf{u}$, the expression (5.2) can be given as

$$\int_{\partial R(t)} (Q\mathbf{n} + Q^A \mathbf{G}_A^T \mathbf{n}) \cdot \mathbf{u} da, \quad (5.6)$$

and correspondingly the configurational entropy flux (5.4). With the use of the transport theorem the principle of irreversibility (5.5) can be obtained in the final form

$$\int_{R(t)} \rho \dot{\eta} dv \geq \int_{R(t)} \rho \theta^{-1} r dv - \int_{\partial R(t)} \{(\theta^{-1} \mathbf{q}) \cdot \mathbf{n} + \theta^{-1} (Q\mathbf{1} + Q^A \mathbf{G}_A^T - \rho \eta \mathbf{1}) \mathbf{n} \cdot \mathbf{u}\} da. \quad (5.7)$$

The invariance with respect to the reparametrization implies furthermore that

$$\theta^{-1} (Q\mathbf{1} + Q^A \mathbf{G}_A^T - \rho \eta \mathbf{1}) = \mathbf{0}, \quad (5.8)$$

and in the absence of microstructure,

$$Q = \rho \eta. \quad (5.9)$$

The result (5.9) was first derived by Fried and Gurtin (1996).

We want to point out that the specific form (5.8) of the configurational heating and its reduced form (5.9) in the case of continua without microstructure have been derived here independently of particular constitutive assumptions.

6. Constitutive equations

The results of the previous section complete the set of general principles of thermodynamics for continua with microstructure and evolving macrodefects and microdefects. They consist of the balance law of mass (2.5), the balance law of macromomentum (2.6), the balance laws of micromomenta (2.7), the balance law

of moment of momentum in the form either (2.8) or (2.9), the balance law of configurational macromomenta and micromomenta (4.1) and (4.2), the balance law of energy (5.3) and the principle of irreversibility (5.7). These laws must be satisfied for all kinds of continua with microstructure and all kinds of continuously distributed and evolving defects. However, these field equations derived from the principles of thermodynamics do not suffice to determine the field variables appearing in them. They must be supplemented by a suitable set of constitutive equations defining particular classes of materials and their interactions with defects evolving in the material.

In order to formulate the constitutive equations various field variables of the balance laws of thermomechanics should be grouped according to the role they play within the considered theory. In general, the variables which are regarded as data of the problem, consist of the set

$$(\rho, \mathbf{f}, \mathbf{f}^4, r). \quad (6.1)$$

The unknown independent field variables, which must be determined from the solution of the problem are

$$(\mathbf{x}, \mathbf{d}_A, \theta), \quad (6.2)$$

while the unknown dependent field variables consisting of

$$(\mathbf{T}, \mathbf{h}^4, \mathbf{T}^4, \mathbf{q}, \psi, \eta) \quad (6.3)$$

must be given by the constitutive equations in terms of the independent field variables (6.2). In the presence of evolving defects there are additionally configurational fields consisting of the configurational macrostress tensor \mathbb{C} and the configurational microstress tensors \mathbb{C}^4 , the configurational momenta \mathbf{p} and \mathbf{p}^4 , and the configurational intrinsic stress vectors \mathbf{f} and \mathbf{f}^4 . The configurational macrostress and microstress tensors are given by the generalized Eshelby relation

$$\mathbb{C} + \mathbf{G}_A^T \mathbb{C}^4 = \{\rho\psi - \frac{1}{2}\rho(\mathbf{v} \cdot \mathbf{v} + \alpha^{AB} \mathbf{w}_A \cdot \mathbf{w}_B)\} \mathbf{1} - (\mathbf{F}^T \mathbf{T} + \mathbf{F}_A^T \mathbf{T}^4), \quad (6.4)$$

while the configurational momenta \mathbf{p} and \mathbf{p}^4 are determined by

$$\mathbf{p} + \mathbf{G}_A^T \mathbf{p}^4 = -(\mathbf{F}^T \mathbf{p} + \mathbf{F}_A^T \mathbf{p}^4), \quad (6.5)$$

where the macromomentum \mathbf{p} and the micromomenta \mathbf{p}^4 are given by Eq. (2.10). On the other hand, the configurational inhomogeneity forces \mathbf{f} and \mathbf{f}^4 are indeterminate in the absence of configurational changes, but otherwise they must be determined by the constitutive equations that govern the kinetics underlying such changes. In view of Eqs. (6.4) and (6.5) the constitutive equations for the intrinsic configurational forces can be obtained from the local form of the balance of configurational forces given as

$$\text{div}(\mathbb{C} + \mathbf{G}_A^T \mathbb{C}^4) + \mathbf{f} + \mathbf{G}_A^T \mathbf{f}^4 = \dot{\mathbf{p}} + \mathbf{G}_A^T \dot{\mathbf{p}}^4. \quad (6.6)$$

It is now seen that the complete set of constitutive equations must be formulated for the field variables (6.3) in terms of the independent variables (6.2).

In general, the constitutive functions are admitted to depend on the independent field variables including their spatial and time derivatives of any order. However, the formal theory of constitutive equations imposes certain restrictions on the admissible form of the constitutive functions. In order to illustrate some essential aspects, we consider here constitutive equations of the following form:

$$\begin{aligned}
\mathbf{T} &= \hat{\mathbf{T}}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}), \\
\mathbf{T}^A &= \hat{\mathbf{T}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}), \\
\mathbf{k}^A &= \hat{\mathbf{k}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}), \\
\Psi &= \hat{\Psi}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}), \\
\mathbf{q} &= \hat{\mathbf{q}}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}), \\
\eta &= \hat{\eta}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta, \nabla \theta; \mathbf{X}),
\end{aligned} \tag{6.7}$$

where $\Psi \equiv \rho\psi$ denotes the free energy measured per unit volume of the reference configuration. The restriction implied by the balance law of (macro)-angular momentum and by the reduced dissipation inequality leads to

$$\begin{aligned}
(\partial_{\mathbf{F}} \hat{\Psi} - \hat{\mathbf{T}}) \cdot \dot{\mathbf{F}} + (\partial_{\mathbf{d}_A} \hat{\Psi} - \hat{\mathbf{k}}^A) \cdot \dot{\mathbf{d}}_A + (\partial_{\nabla \mathbf{d}_A} \hat{\Psi} - \hat{\mathbf{T}}^A) \cdot \nabla \dot{\mathbf{d}}_A + (\partial_{\dot{\mathbf{d}}_A} \hat{\Psi}) \cdot \ddot{\mathbf{d}}_A \\
+ (\partial_{\theta} \hat{\Psi} - \hat{\eta}) \dot{\theta} + (\partial_{\nabla \theta} \hat{\Psi}) \cdot \nabla \dot{\theta} + \theta^{-1} \mathbf{q} \cdot \nabla \theta \leq 0
\end{aligned} \tag{6.8}$$

for every admissible thermodynamical process (in the quasi-static case the microinertia terms may be omitted). It is seen now, that the free energy function $\hat{\Psi}$ may neither depend on $\dot{\mathbf{d}}_A$ nor on $\nabla \theta$, i.e. the most general first order form of the free energy is

$$\Psi = \hat{\Psi}(\mathbf{F}, \mathbf{d}_A, \nabla \mathbf{d}_A, \theta). \tag{6.9}$$

Moreover, the constitutive functions for the macrostress tensor \mathbf{T} and the microstress vector \mathbf{T}^A are completely determined by the free energy function, i.e.

$$\begin{aligned}
\mathbf{T} &= \hat{\mathbf{T}}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B) = \partial_{\mathbf{F}} \hat{\Psi}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \theta), \\
\mathbf{T}^A &= \hat{\mathbf{T}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B) = \partial_{\nabla \mathbf{d}_A} \hat{\Psi}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \theta),
\end{aligned} \tag{6.10}$$

and the entropy is given by

$$\eta = \hat{\eta}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}, \theta) = \partial_{\theta} \hat{\Psi}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}, \theta). \tag{6.11}$$

Thus, only the intrinsic microstress \mathbf{k}^A can depend on $\dot{\mathbf{d}}_A$, and the most general first order constitutive equation for \mathbf{k}^A has the form

$$\mathbf{k}^A = \partial_{\dot{\mathbf{d}}_A} \hat{\Psi}(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \theta) + \bar{\mathbf{k}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B, \theta), \tag{6.12}$$

where the constitutive function $\bar{\mathbf{k}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B)$ must satisfy the following restriction:

$$\bar{\mathbf{k}}^A(\mathbf{F}, \mathbf{d}_B, \nabla \mathbf{d}_B, \dot{\mathbf{d}}_B) \cdot \dot{\mathbf{d}}_C \geq 0. \tag{6.13}$$

The constitutive relations for the configurational forces can now be obtained from Eq. (6.6), which can be rewritten as

$$\mathbf{f} + \mathbf{G}_A^T \mathbf{f}^A = \dot{\mathbf{p}} + \mathbf{G}_A^T \dot{\mathbf{p}}^A - \operatorname{div}(\mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A), \tag{6.14}$$

where

$$\mathbb{C} + \mathbf{G}_A^T \mathbb{C}^A = \{\hat{\Psi} - \frac{1}{2} \rho (\mathbf{v} \cdot \mathbf{v} + \alpha^{AB} \mathbf{w}_A \cdot \mathbf{w}_B)\} \mathbf{1} - (\mathbf{F}^T \hat{\mathbf{T}} + \mathbf{F}_A^T \hat{\mathbf{T}}^A), \tag{6.15}$$

with the constitutive functions for $\hat{\Psi}$, $\hat{\mathbf{T}}$ and $\hat{\mathbf{T}}^A$ given by Eqs. (6.9) and (6.10), respectively. Thus, substituting Eqs. (6.9) and (6.10) into Eq. (6.15) and subsequently into Eq. (6.14) and performing the required differentiation the constitutive relation for the inhomogeneity forces \mathbf{f} and \mathbf{f}^A are obtained.

The constitutive equations derived above are restricted further by the principle of material frame-indifference and possible material symmetries. The final form of such constitutive equations can be obtained then by standard procedures.

7. Discussion and closing remarks

In this paper we present a framework for the analysis of continua with microstructure and evolving defects on the macrolevel and microlevel. The balance laws for deformational and configurational macro-forces and microforces are derived and the first and second law of thermodynamics are presented taking into account inertia effects and the dissipation of the evolving macrodefects and microdefects. To close the set of equations, which enables the analysis of continua with defect evolution, we present finally the most general form of the first order constitutive equations.

Within the framework of this paper various special models of continua with microstructure and evolving defects can be obtained by introducing simplifying assumptions concerning the number of the directors and the type of their deformation according to the class of materials under consideration. In this way e.g. Cosserat continua and continua with three deformable directors, representing the orientation of the crystal lattice, can be derived for problems with changing microstructure and migration of defects on the macrolevel and microlevel.

Further investigations should take into account the evolution of distinguished cracks on singular surfaces (singular lines in the two-dimensional case). Also the derivation of phenomenological damage models from the presented microtheories by introducing appropriate plastic and/or damage potentials should be considered.

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