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Thermodynamics of Deformable Dielectrics with a Non-Euclidean Structure as Internal Variable

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In this paper we apply the geometrical theory of thermodynamics with vectorial and tensorial internal variables to a model of deformable dielectrics (which include ferro-electric crystals) due to Maugin. We explicitly consider an internal (non-Euclidean) metric as a thermodynamical non-equilibrium variable, together with polarization and temperature gradients. With the aid of Clausius-Duhem inequality we obtain the extra entropy flux and the relevant thermodynamical restrictions on entropy and free energy.

1 Introduction

In recent years there has been extensive work on a model for a fully Galilean thermo-electrodynamics of dielectric deformable media proposed by Maugin and co-workers in a series of papers (Maugin and Pouget, 1980; Maugin, 1976, 1977a,b, 1988). This general non-linear model is based on an extensive application of the principle of virtual power to continuum thermo-mechanics in presence of electromagnetic fields, as developed by the French school (Maugin, 1980). The models considered in the literature quoted above include all kinds of deformable dielectrics and in particular they have revealed themselves to be useful in explicit calculations involving models of ferro-electric crystals and piezoelectricity. The concrete applicative interest of these theoretical models resides in their explicit application to genuine materials important for technology, like the chemical components of polarizable crystals used in electronic devices as, e.g., the barium titanate of the Perowskity family, see Kittel (1966).

1.1 The General Model for Deformable Dielectrics

We shall first summarize the theoretical framework developed by Maugin and coworkers in Maugin and Pouget (1980); Maugin (1976, 1977a,b, 1980, 1988) to which we refer the reader for further details and examples of applications. The considered model takes into account the stringent hypothesis that in nature there exist continua in which elasto-mechanics phenomena couple with electro-magnetic phenomena encoded into constitutive equations which depend on the electric polarization as well as on its spatial gradient. The thermodynamical properties of these continua in situations far from equilibrium (i.e. when the temperature varies non-uniformly together with its spatial gradient) lead to extra contributions into the Clausius-Duhem inequality (see Müller (1985); Maugin (1990)) related to extra terms in the entropy flux. Following Maugin (see e.g. Eringen and Maugin (1989)) we consider a body $\mathbb{B}$ with regular boundary $\partial\mathbb{B}$, which is continuously embedded into the Euclidean 3-space $\mathbb{R}^3$ by means of a family of time-dependent configurations. The mechanical properties of the body are encoded by a *density function* μ, the *deformation gradient* $\mathbf{F}$ (which is assumed to be invertible with inverse $\mathbf{F^{-1}}$), the *symmetric Cauchy stress-tensor* $\mathbf{T}$, the *internal energy* per unit mass e and the *rate of deformation*

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F^{-1}}. \tag{1}$$

The thermomechanical properties of the body are encoded into the *temperature field* θ (together with its spatial gradient $\nabla\theta$), the *heat flux* $\mathbf{q}$, the *entropy function* S and the *entropy flux* $\mathbf{J}_S$. The electromagnetic properties of the body are reflected into an internal electric field vector ${}^L\mathbf{E}$ and a second order tensor ${}^L\mathbb{E}$. The first is called the *local electric-field vector* and it accounts for the interaction between the polarization of "different molecular species" and the usual crystal lattice; the tensor ${}^L\mathbb{E}$ is called *shell-shell interaction tensor* and accounts for polarization gradients. The *vector polarization* per unit of mass is denoted by $\boldsymbol{\pi}$ and its gradient is $\nabla\boldsymbol{\pi}$. The body is embedded into an *ambient electromagnetic field* with components $(\mathbf{E}, \mathbf{B})$. According to Maugin and Pouget (1980) a Galilean quasi-static approximation is chosen in which

$$\boldsymbol{\mathcal{E}} = \mathbf{E} + \mathbf{c^{-1}}\mathbf{U} \times \mathbf{B} \tag{2}$$

is the electric field in a co-moving frame (here c is the velocity of light in vacuum). Denoting by $p_{(i)}$ the *virtual power of internal forces*, the balance equation of the model turns out to be

$$p_{(i)} = \mathbf{T} \cdot \mathbf{D} - \mu {}^L\mathbf{E} \cdot \hat{\boldsymbol{\pi}} + {}^L\mathbb{E} \cdot \hat{\nabla \boldsymbol{\pi}} \tag{3}$$

(see e.g. Maugin and Pouget (1980) eqn. (48)), where: the symbol $\cdot$ denotes full tensor contraction; $\mathbf{D}$ is the symmetric part of $\mathbf{L}$ ($\mathbf{T} \cdot \mathbf{D}$ is in fact equal to $\mathbf{T} \cdot \mathbf{L}$ because of the symmetry of $\mathbf{T}$); the hat $\hat{}$ denotes the so-called *Jaumann "co-rotational derivative"* operator, defined by the local formula

$$\hat{\zeta}_i = \dot{\zeta}_i - \Omega_{ik}\zeta_k, \tag{4}$$

where ζ_i are the Cartesian components of a vector field $\boldsymbol{\zeta}$, the $\dot{}$ denotes total time derivative, $\boldsymbol{\Omega}$ is the rotational part of $\mathbf{L}$ ($2\Omega_{ij} = L_{ij} - L_{ji}$) and summation over repeated indices is understood. Whenever non-rotating frames are chosen ($\boldsymbol{\Omega} = 0$) eqn. (3) reduces to the simpler expression

$$p_{(i)} = \mathbf{T} \cdot \mathbf{D} - \mu {}^L\mathbf{E} \cdot \dot{\boldsymbol{\pi}} + {}^L\mathbb{E} \cdot \dot{\nabla \boldsymbol{\pi}}. \tag{5}$$

The dynamical behaviour of the polarization field $\boldsymbol{\pi}$ is encoded into the following equation

$$\boldsymbol{\mathcal{E}} + {}^L\mathbf{E} + \mu^{-1} div({}^L\mathbb{E}) = d\ddot{\boldsymbol{\pi}} \tag{6}$$

(eqn. (55) of Maugin and Pouget (1980)), where $div({}^L\mathbb{E}) = \nabla \cdot {}^L\mathbb{E}$ is locally given by ${}^L\mathbb{E}_{ik,j}$ and $d \neq 0$ is a coefficient which expresses the so-called *polarization inertia*. In the sequel we shall use units for which $d = 1$. The first principle of thermodynamics in integral form reads (see Maugin and Pouget (1980) eqns. (33)-(46))

$$\begin{aligned} &\frac{d}{dt}\Big[\int_{\mathbb{B}_t} \frac{1}{2}\mu(\mathbf{U}^2 + d\dot{\boldsymbol{\pi}}^2)dV + \int_{\mathbb{B}_t} \mu e dV + \int_{\mathbb{B}_t} \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)dV\Big] = \\ &= \int_{\mathbb{B}_t} \mathbf{f} \cdot \mathbf{U} dV + \int_{\partial\mathbb{B}_t} (\boldsymbol{\tau} \cdot \mathbf{U} + \mu \boldsymbol{\pi}_S \cdot \dot{\boldsymbol{\pi}}) da + \\ &+ \Big[\int_{\mathbb{B}_t} \mu h dV - \int_{\partial\mathbb{B}_t} \mathbf{q} \cdot \mathbf{n} da\Big], \end{aligned} \tag{7}$$

where: $\mathbb{B}_t$ is the actual configuration; $\mathbf{U}$ is the *velocity field* of the body; e is the *internal energy* per unit of mass; $\mathbf{f}$ is the *body force*; $\boldsymbol{\tau}$ is the *surface traction* of purely mechanical origin ; $\boldsymbol{\pi}_S$ is the *surface density* of electric dipoles; h is the *heat radiation* per unit of mass; $\mathbf{n}$ is the outer normal of $\partial\mathbb{B}_t$; dV and da denote the volume and the surface elements. The second principle of thermodynamics in integral form reads as follows

$$\frac{d}{dt}\int_{\mathbb{B}_t} \mu S dV - \int_{\mathbb{B}_t} \mu\sigma dV + \int_{\partial\mathbb{B}_t} \mathbf{J}_S \cdot \mathbf{n} da \geq 0, \tag{8}$$

where σ is the *entropy source* per unit of mass. Starting from equation (7) the local equation for $\dot{e}$ is obtained in Maugin and Pouget (1980) (eqn. (65)) under the form

$$\mu\dot{e} = p_{(i)} - \nabla \cdot (\mathbf{q} - \mathbf{P}) + \mu h, \tag{9}$$

where $\mathbf{P}$ is the Poynting vector. By means of a Legendre transformation, one introduces then the free energy Ψ as follows

$$\Psi = e - \theta S. \tag{10}$$

In Maugin and Pouget (1980) the following constitutive relations are chosen for σ and $\mathbf{J}_S$:

$$\sigma = \frac{h}{\theta},\ \mathbf{J}_S = \frac{\mathbf{q} - \mathbf{P}}{\theta}. \tag{11}$$

Starting from the second principle of thermodynamics and using equations (10) and (11) one finally obtains the Clausius-Duhem inequality under the form

$$-\mu(\dot{\Psi} + S\dot{\theta}) + p_{(i)} - \frac{1}{\theta}(\mathbf{q} - \mathbf{P}) \cdot \nabla\theta \geq 0. \tag{12}$$

In the following we will not take into consideration the vector $\mathbf{P}$. For further details and explicit applications we refer the reader to Maugin and Pouget (1980) and references quoted therein.

1.2 The Geometrical Perspective on Internal Variables

In a series of recent papers (see Dolfin et al. (1998a); Francaviglia et al. (2002)) two of us have developed and applied with other authors a geometric method to deal with elasto-thermomechanical systems endowed with scalar, vector and tensor internal variables, even including among them local non-Euclidean metrics of thermomechanical origin (see Valanis (1995)). The purpose of this paper is to apply these new techniques to the model described in Subsection 1.1. Before doing this we shall thence summarize the idea. The geometrical framework was developed in Dolfin et al. (1998a, 1999) on the basis of earlier ideas of Coleman and Owen (Coleman and Owen, 1974; Owen, 1984). It was there considered a state space at time t as the set B_t of all state variables which "fit" the configuration of any single material element at time t. The set B_t is assumed to have the structure of a finite dimensional manifold so that the "total state space" is given by the disjoint union

$$\mathcal{B} = \bigcup_t \{t\} \times B_t \tag{13}$$

with a given natural structure of fibre bundle over the real line $\mathbb{R}$ where time flows (Dolfin et al., 1998a, 1999). This idea comes from the "homogeneous formalism" of classical mechanics (or from relativistic considerations if one prefers) and allows to treat also the time variable on an equal footing with the other thermodynamical parameters. The justification is deeply rooted into the purpose of applying the technique to situations far from equilibrium and of dissipative non-reversible nature, in which time cannot be frozen and it plays a dominant role in a sense equivalent to the entropy role according to the second principle. If the instantaneous state space B_t does not vary in time the total state space $\mathcal{B}$ reduces to the Cartesian product $\mathbb{R} \times B$. Moreover, it was considered an abstract space of processes (Dolfin et al., 1998a, 1999; Coleman and Owen, 1974; Owen, 1984; Noll, 1958) which consists of a set π of functions

$$P_t^i : [0, t] \to G, \tag{14}$$

where $[0, t]$ is any time interval, the space G is a suitable target space suggested by the model, i is a label ranging in an unspecified index set for all allowed processes and $t \in \mathbb{R}$ is the so called *duration of the process*. A continuous function

$$\rho : \mathbb{R} \to C^0(B_0, B_t) \tag{15}$$

is defined in Dolfin et al. (1999); Coleman and Owen (1974); Owen (1984); Noll (1958) so that for any instant of time t and for any process $P_t^i \in \pi$ a continuous mapping called *transformation* (induced by the process) is generated. It is known that a real process occurs outside equilibrium and thermodynamical theories describing transformations of this kind are known as non-equilibrium theories (De Groot and Mazur, 1962). They consist in describing the system in such a state of non-equilibrium using the same state space which already accounted for the equilibrium state variables.

In some cases, however, the description of the evolution of a thermodynamical system requires an extension of the state space through the introduction of further dynamical variables like, for instance, internal variables. Internal variables represent micro-local or mesoscopic phenomena which one cannot control in full detail and can be described as averages governed by a set of parameters (of mechanical, thermodynamical or other physical origin) having a mathematical structure which is suggested by the particular model chosen for the continuum (see De Groot and Mazur (1962); Verhas (1997); Muschik (1990) for the general theory and applications). In principle and for simplicity one assumes that the internal variables are collectively denoted by $\boldsymbol{\alpha}$, a variable which ranges in a suitable vector space. In particular we shall be concerned in cases in which this vectorial space contains scalars, vector fields and tensor fields over the body $\mathbb{B}$.

Following Dolfin et al. (1999) we assume that our body $\mathbb{B}$ is mechanically a "simple material" (in the sense of Noll (1958)) endowed with internal variables of thermodynamic and electromagnetic origin. As in eqn. (30) of Dolfin et al. (1998a) the state space B is assumed as the direct sum

$$B = Lin(\nu) \oplus \mathbb{R} \oplus \nu \oplus W \oplus Lin(W), \tag{16}$$

where $\nu \simeq \mathbb{R}^3$ and W is the space of all internal variables. In Dolfin et al. (1998a) the variables of B were denoted by $(\mathbf{F}, e, \boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\nabla\alpha})$ where: $\boldsymbol{\beta} = grad\theta$ is proportional to the gradient of the temperature θ. The process is described by the assignment of a piecewise continuous function $P_t = [\mathbf{L}(t), f(t), \boldsymbol{\gamma}(t)]$, where $\mathbf{L}$ is the rate of deformation as in eqn. (1), $f(t) = -div\mathbf{q}$ and $\boldsymbol{\gamma}$ is a phenomenological function accounting for the non uniformity in time of the gradient of temperature. The dynamical system associated with the process was assumed in Dolfin

et al. (1998a) to be the following

$$\begin{cases} \dot{\mathbf{F}} = \mathbf{L}\mathbf{F} \\ \mu\dot{e} = \mathbf{T} \cdot Ł + f \\ \dot{\nabla\theta} = \boldsymbol{\gamma} \\ \dot{\boldsymbol{\alpha}} = \nabla \cdot \mathbf{J}_{\boldsymbol{\alpha}} + \sigma_{\boldsymbol{\alpha}}, \end{cases} \tag{17}$$

where $\mu \neq 0$ is the density of mass; $\mathbf{T}$ is the Cauchy stress tensor as above, while $\mathbf{J}_{\boldsymbol{\alpha}}$ and $\sigma_{\boldsymbol{\alpha}}$ are the internal variable flux and the internal variable source respectively (see Dolfin et al. (1998a)).

Following the method of Coleman and Owen (1974), in Dolfin et al. (1998a) it is shown that the entropy action $s(\rho_t, b, t)$ is defined in terms of its variables ρ_t (the thermodynamic transformation induced by the process), b (the initial state) and t (time) by an expression of the following kind

$$\begin{aligned} s(\rho_t, b, t) &= -\int_0^t \frac{1}{\mu}\nabla \cdot \mathbf{J}_S dt = \\ &= \int_0^t \frac{h}{\mu\theta}dt + \int_0^t \frac{1}{\mu\theta^2}(\mathbf{q} \cdot \boldsymbol{\beta})dt - \int_0^t \frac{1}{\mu}\nabla \cdot \mathbf{k}dt, \end{aligned} \tag{18}$$

where the total entropy flux $\mathbf{J}_S$ is phenomenologically assumed to have the form

$$\mathbf{J}_S = \frac{\mathbf{q}}{\theta} + \mathbf{k}, \tag{19}$$

being $\mathbf{k}$ an *extra flux of entropy* due to dissipation out of equilibrium (as introduced in Müller (1985) or in Maugin (1990)). Notice that assuming (19) instead of the simpler relation $\mathbf{J}_S = \frac{\mathbf{q}}{\theta}$ as in $(11)_2$ above (with $\mathbf{P} = 0$) produces extra terms into the correspondig Clausius-Duhem inequality.

One assumes then that the system under consideration admits an "upper potential" (in the sense of Coleman and Owen (1974); Owen (1984)), i.e. an entropy function S which satisfies

$$S(b_t) - S(b) \geq s(\rho_t, b, t)$$

for all processes. Thence the entropy satisfies the second law under the form

$$\mu\dot{S} + \nabla \cdot \mathbf{J}_S \geq 0, \tag{20}$$

or equivalently

$$\mu\theta\dot{S} + \nabla \cdot (\theta\mathbf{J}_S) - (\mathbf{J}_S \cdot \nabla)\theta \geq 0 \tag{21}$$

for $\theta \geq 0$. It is then convenient to replace the internal energy e with its Legendre transform $\Psi = e - \theta S$, as in eqn. (10). The free energy is assumed to satisfy a constitutive ansatz of the type

$$\Psi = \Psi(\mathbf{F}, \boldsymbol{\beta}, \boldsymbol{\alpha}, \nabla\boldsymbol{\alpha}) \tag{22}$$

and the extra flux is postulated to follow the phenomenological ansatz

$$\mathbf{k} = \frac{1}{\theta}\mathbf{B} \cdot \dot{\boldsymbol{\alpha}} \tag{23}$$

with

$$\mathbf{B} = -\frac{\partial\Psi}{\partial(\nabla\boldsymbol{\alpha})}. \tag{24}$$

Out of these hypothesis one can specify the form of the gradient of deformation $\mathbf{F}$, in order to exploit (18) in terms of $\mathbf{k}$ and in order to work out the explicit form of the Clausius-Duhem inequality together with its thermodynamical restrictions on the process.

As a concrete specific example, in Dolfin et al. (1998a,b) we considered the case in which $\mathbf{F}$ admits an additive decomposition $\mathbf{F} = \mathbf{F}^e + \mathbf{F}^i$ or a "Lee decomposition" $\mathbf{F} = \mathbf{F}^e\mathbf{F}^i$, where the elastic part $\mathbf{F}^e$ replaces explicitly $\mathbf{F}$ and the inelastic part $\mathbf{F}^i$ takes the role of a tensorial internal variable. The relevant equations are then equations (51) and (55) of Dolfin et al. (1998a), to which we refer the reader for further details. In a further paper (Francaviglia et al., 2002) it was instead considered the possibility of introducing as extra internal variable an "inner metric" $\mathbf{g}$ which mixes up with the deformation gradient $\mathbf{F}$ through an algebraic relation of the type

$$\mathbf{C} = \mathbf{F}^T\mathbf{g}\mathbf{F}, \tag{25}$$

where $\mathbf{C}$ is the material *Cauchy-Green tensor* and $\mathbf{F}^T$ denotes the transpose. The internal variable $\mathbf{g}$ is a non -Euclidean metric tensor that has to do with an average tensor characterization of local deviations from the Euclidean structure associated with effects on the mesoscopic scale (atomic, molecular or grain level), see Valanis (1995). What we mean is that if the microscopic subdomains have characteristic dimension too small to be detected by technical instruments of measure then one may only observe the motion of certain aggregates of microscopic subdomains. We call these detectable subsets *mesoscopic subdomains*. Along a thermodynamical process the individual microdomains migrate and diffuse, so that a domain's neighborhood is constantly changing. This micromotion may influence the topology of the body, resulting thus in a non-affine deformation superposed on the deformation of a mesodomain (Ciancio et al., 2001). This additional effect gives rise to a non-Euclidean (local) structure. Moreover, it can produce an additional dissipation of energy inside the body which is not due to macroscopic phenomena. We take into account this type of situation by regarding the physical metric as an internal variable. Then if, accordingly, we use (25) as a generalization of Cauchy-Green tensor, the relevant equations turn out to be relations (25)-(30) and (38)-(40) of Francaviglia et al. (2002).

2 A New Model of Elastic Deformable Dielectrics with an Internal Metric

In this Section we are finally ready to apply the techniques of Dolfin et al. (1998a), Francaviglia et al. (2002) as summarized in Subsection 1.2 to the general model of Maugin recalled in Subsection 1.1. The state space B is now given by eqn. (16) where the space W of internal variables accounts now for both an internal metric $\mathbf{g}$ of thermodynamical origin (as in Francaviglia et al. (2002)) and for the electric polarization vector $\boldsymbol{\pi}$. In other words we assume

$$W = \nu \oplus Met(\nu), \tag{26}$$

where $Met(\nu)$ denotes the space of all metric tensors on the vector space $\nu \simeq \mathbb{R}^3$ mechanically associated to the body. To be more precise, $\boldsymbol{\pi}$ should be rather considered as a state variable depending on the internal variables ${}^L\mathbf{E}$ and ${}^L\mathbb{E}$ through eq. (6). However there is no change if, for simplicity, we treat formally $\boldsymbol{\pi}$ as an internal variable. Finally we recall that as in the previous paper Francaviglia et al. (2002), the internal variable $\mathbf{g}$ and the mechanical variable $\mathbf{F}$ mix up according to eqn. (25). As a result, under these hypotheses the theory can be formally and more conveniently re-written on the new state space

$$\hat{B} = Lin(\nu \oplus \nu) \oplus \mathbb{R} \oplus \nu \oplus [\nu \oplus Lin(\nu)] \tag{27}$$

having obviously embedded $Met(\nu)$ into $Lin(\nu)$. In other words we split $\mathbf{C}$ and assume our variables to be

$$(\mathbf{F}, \mathbf{g}, e, \nabla\theta, \boldsymbol{\pi}, \nabla\boldsymbol{\pi})$$

which live in the space $\hat{B}$ of (27). Alternatively, if we prefer not to split $\mathbf{C}$ thence we assume as variables the following

$$(\mathbf{C}, e, \nabla\theta, \boldsymbol{\pi}, \nabla\boldsymbol{\pi})$$

with $\mathbf{C}$ given by (25), which live in the further space

$$\tilde{B} = Lin(\nu) \oplus \mathbb{R} \oplus \nu \oplus [\nu \oplus Lin(\nu)]. \tag{28}$$

Moreover, no dependence whatsoever on $\nabla\mathbf{g}$ will be considered, since covariant effects associated with the metric should in fact pass through higher order derivatives of $\mathbf{g}$ involved in curvature (see, e.g., Valanis (1995)). This kills the component $Lin[Met(\nu)]$ from the effective dynamical variables.

We are now ready to work on the problem of finding expressions for $\mathbf{L}$, its symmetric part $\mathbf{D}$ and the quantity $\mathbf{T} \cdot \mathbf{D}$ which enters eqn. (3) for $p_{(i)}$. Notice first that we are facing an implicit function problem, hidden in the fact that among the three variables $\mathbf{F}$, $\mathbf{g}$ and $\mathbf{C}$ only two are independent because of eqn. (25). Specific calculations suggest us to choose the two independent variables in different ways depending upon the formula envisaged (e.g., to calculate $\mathbf{L}$, $\mathbf{T} \cdot \mathbf{D}$ and the entropy different but equivalent choices lead to simpler formulae). Here we deal directly use the various results, the derivation of which is postponed to a technical appendix. Because of (10), nothing will change if the internal energy e is replaced by θ as an equivalent state variable. Using the relations derived in the appendix, we see that a convenient choice for the dynamical system associated with the process and

replacing (17) is the following

$$\begin{cases} \dot{\mathbf{C}} = \mathbf{F}^T[\mathbf{g}^{-1}\mathbf{L}^{\mathbf{T}}\mathbf{g} + \mathbf{L} + \mathbf{g}^{-1}\dot{\mathbf{g}}]\mathbf{F} \\ \mu\dot{e} = p^{(i)} - \nabla\cdot\mathbf{q} \\ \dot{\nabla\theta} = \nabla\cdot\mathbf{J}_{\nabla\theta} + \sigma_{\nabla\theta} \\ \dot{\boldsymbol{\pi}} = \int_0^t (\boldsymbol{\mathcal{E}} + {}^L\mathbf{E} + \mu^{-1}div({}^L\mathbb{E}))d\tau \\ \dot{\nabla\boldsymbol{\pi}} = \nabla\cdot\mathbf{J}_{\nabla\boldsymbol{\pi}} + \boldsymbol{\sigma}_{\boldsymbol{\nabla\pi}} \\ \dot{\mathbf{g}} = \mathbf{G}(t), \end{cases} \tag{29}$$

where $\mathbf{J}_{\nabla\theta}$, $\mathbf{J}_{\nabla\boldsymbol{\pi}}$, $\boldsymbol{\sigma}_{\nabla\theta}$ and $\boldsymbol{\sigma}_{\nabla\boldsymbol{\pi}}$ are the current vectors and the sources of the gradient of the temperature and the gradient of polarization respectively. In the next Section we will show, by suitable thermodynamical considerations, how the splitting (25) of $\mathbf{C}$ into the gradient of deformation $\mathbf{F}$ and the physical metric $\mathbf{g}$, using equation $(29)_1$ as a necessary condition, reflects into the dissipation inequality.

3 Exploitation of the Dissipation Inequality

According to our hypothesis above, the free energy is then given as a functional of the type

$$\Psi = \Psi(\mathbf{C}, \boldsymbol{\pi}, \nabla\boldsymbol{\pi}, \theta, \nabla\theta). \tag{30}$$

By derivation with respect to time one obtains

$$\dot{\Psi} = \tilde{\mathbf{T}}\cdot\dot{\mathbf{C}} + \mathbf{H}\cdot\dot{\boldsymbol{\pi}} + \mathbf{Y}\cdot(\dot{\nabla\boldsymbol{\pi}}) - \tilde{s}\dot{\theta} + \mathbf{R}\cdot(\dot{\nabla\theta}), \tag{31}$$

where the following positions are made

$$\tilde{\mathbf{T}} = \frac{\partial\Psi}{\partial\mathbf{C}};\ \ \mathbf{H} = \frac{\partial\Psi}{\partial\boldsymbol{\pi}};\ \ \mathbf{Y} = \frac{\partial\Psi}{\partial(\nabla\boldsymbol{\pi})};\ \ \tilde{s} = -\frac{\partial\Psi}{\partial\theta};\ \ \mathbf{R} = \frac{\partial\Psi}{\partial(\nabla\theta)}. \tag{32}$$

Formally, the pair $(\boldsymbol{\pi}, \theta)$ can be seen as a single internal variable $\boldsymbol{\alpha}$, so that the pair $(\mathbf{Y}, \mathbf{R})$ corresponds to $\mathbf{B}$ as given by eqn. (24). After some simple manipulation, the following form of equation (31) is obtained

$$\dot{\Psi} = \tilde{\mathbf{T}}\cdot\dot{\mathbf{C}} + \mathcal{A}\cdot\dot{\boldsymbol{\pi}} + \frac{\partial\Psi}{\partial\theta}\dot{\theta} + \nabla\cdot(\mathbf{Y}^T\cdot\dot{\boldsymbol{\pi}}) + \mathbf{R}\cdot\left(\dot{\nabla\theta}\right), \tag{33}$$

where

$$\mathcal{A} = \frac{\partial\Psi}{\partial\boldsymbol{\pi}} - \nabla\cdot\left[\frac{\partial\Psi}{\partial(\nabla\boldsymbol{\pi})}\right] = \frac{\delta\Psi}{\delta\boldsymbol{\pi}}$$

is the variational derivatives of Ψ with respect to the state variable $\boldsymbol{\pi}$. From the first and the second principle of thermodynamics

$$\begin{cases} \mu\dot{e} = p_{(i)} - \nabla\cdot\mathbf{q} \\ \mu\dot{S} + \nabla\cdot\mathbf{J}_S \geq 0, \end{cases} \tag{34}$$

where S is the entropy per unit mass, one obtains the general form for the Clausius-Duhem inequality

$$-\mu(\dot{\Psi} + S\dot{\theta}) + p_{(i)} + \nabla\cdot(\theta\mathbf{k}) - \mathbf{J}_S\cdot\nabla\theta \geq 0, \tag{35}$$

when the extra entropy flux $\mathbf{k}$ given by (19) is considered. In the model developed in Maugin (1980) the power of internal forces is explicitly given by (5). Easy manipulations (see eqn.(59) of the appendix) give

$$\mathbf{L} = \mathbf{M}^{-\mathbf{1}}(\dot{\mathbf{C}}\mathbf{C}^{-\mathbf{1}})\mathbf{M} - \mathbf{M}^{-\mathbf{1}}\dot{\mathbf{M}} \tag{36}$$

with

$$\mathbf{M} = \mathbf{F}^T\mathbf{g} = \mathbf{C}\mathbf{F}^{-1}. \tag{37}$$

Recalling then that $\mathbf{D}$ is the symmetric part of the velocity gradient $\mathbf{L}$, one obtains from (5) and (36) the following explicit expression for the power of internal forces in our model

$$\begin{aligned} p_{(i)} \quad = \quad & -\mathbf{Z}\cdot\dot{\mathbf{M}} + \left(\mathbf{Z}\mathbf{F}^{-T}\right)\cdot\dot{\mathbf{C}} + \\ & -\mu^L\mathbf{E}\cdot\dot{\boldsymbol{\pi}} + {}^L\mathbb{E}\cdot\dot{\nabla\boldsymbol{\pi}}, \end{aligned} \tag{38}$$

where we set for simplicity $\mathbf{Z} \equiv \mathbf{M}^{-T}\mathbf{T} = (\mathbf{T}\mathbf{M}^{-1})^T$; the notation $\mathbf{X}^{-T} = (\mathbf{X}^{-1})^T$ is used for all matrices $\mathbf{X}$.

By substituting equation (38) into the Clausius-Duhem inequality, the following relation is obtained

$$\begin{aligned} - \quad & \mu(\dot{\Psi} + S\dot{\theta}) - \mathbf{Z}\cdot\dot{\mathbf{M}} + \left(\mathbf{Z}\mathbf{F}^{-T}\right)\cdot\dot{\mathbf{C}} + \\ - \quad & \mu\,{}^{L}\mathbf{E}\cdot\dot{\boldsymbol{\pi}} + {}^{L}\mathbb{E}\cdot\dot{\nabla\boldsymbol{\pi}} + \nabla\cdot(\theta\mathbf{k}) - \mathbf{J}_S\cdot\nabla\theta \geq 0. \end{aligned} \tag{39}$$

We now replace equation (31) into equation (39) and obtain

$$\begin{aligned} & (\mathbf{Z}\mathbf{F}^{-T} - \mu\tilde{\mathbf{T}})\cdot\dot{\mathbf{C}} - \mu(\mathcal{A} + {}^{L}\mathbf{E})\cdot\dot{\boldsymbol{\pi}} + \\ & + {}^{L}\mathbb{E}\cdot\dot{\nabla\boldsymbol{\pi}} - \mu(\frac{\partial\Psi}{\partial\theta} + S)\dot{\theta} + \\ & -\mathbf{Z}\cdot\dot{\mathbf{M}} + \mu\nabla\cdot\Big[\frac{\theta\mathbf{k}}{\mu} - \mathbf{Y}^T\dot{\boldsymbol{\pi}}\Big] + \mathbf{R}\cdot\dot{\nabla\theta} + \frac{1}{\mu}\theta\mathbf{k}\cdot\nabla\mu - \mathbf{J}_S\cdot\nabla\theta \geq 0. \end{aligned} \tag{40}$$

From inequality (40) the following constitutive relations are obtained

$$\tilde{\mathbf{T}} = \frac{\partial\Psi}{\partial\mathbf{C}} = \mu^{-1}\mathbf{Z}\mathbf{F}^{-T}, \tag{41}$$

$$\frac{\partial\Psi}{\partial\theta} = -S, \quad \frac{\partial\Psi}{\partial(\nabla\theta)} = 0, \tag{42}$$

$$\mathcal{A} = -{}^{L}\mathbf{E}, \tag{43}$$

$$\mathbf{k} = \frac{\mu}{\theta}\Big[\Big(\frac{\partial\Psi}{\partial(\nabla\boldsymbol{\pi})}\Big)^T\dot{\boldsymbol{\pi}}\Big]. \tag{44}$$

Then the following dissipation inequality remains

$$-\mathbf{Z}\cdot\dot{\mathbf{M}} + {}^{L}\mathbb{E}\cdot\dot{\nabla\boldsymbol{\pi}} + \frac{1}{\mu}\theta\mathbf{k}\cdot\nabla\mu - \mathbf{J}_S\cdot\nabla\theta \geq 0. \tag{45}$$

3.1 Exploitation of the Entropy Action

We now exploit the expression for the entropy action already defined in section 1.1 (see equation (18) for our model). By using the first principle of thermodynamics $(34)_1$ together with the explicit expression for the power of internal forces (38) one obtains

$$-\nabla\cdot\mathbf{q} = \mu\dot{e} + \mathbf{Z}\cdot\dot{\mathbf{M}} - \left(\mathbf{Z}\mathbf{F}^{-T}\right)\cdot\dot{\mathbf{C}} + \mu\,{}^{L}\mathbf{E}\cdot\dot{\boldsymbol{\pi}} - {}^{L}\mathbb{E}\cdot\dot{\nabla\boldsymbol{\pi}}. \tag{46}$$

By substituting equation (46) into (18) the explicit expression for the entropy action along the transformation for the system is obtained

$$\begin{aligned} s \quad = \quad & \int_\sigma \frac{1}{\theta}de - \frac{\mathbf{Z}\mathbf{F}^{-T}}{\mu\theta}\cdot d\mathbf{C} + \left[\frac{{}^{L}\mathbf{E}}{\theta} - \frac{1}{\mu}\nabla\cdot\left(\frac{\mu\mathbf{Y}}{\theta}\right)\right]\cdot d\boldsymbol{\pi} + \\ - \quad & \frac{1}{\theta}\left(\frac{{}^{L}\mathbb{E}}{\mu} + \mathbf{Y}\right)\cdot d\left(\nabla\boldsymbol{\pi}\right) + \frac{1}{\mu\theta}\left[\mathbf{Z}\cdot\dot{\mathbf{M}} + \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta\right]dt, \end{aligned} \tag{47}$$

so that the entropy function is now calculated as an integral along a path σ into the appropriate space $\mathbb{R}\times\mathcal{B}^*$ of all thermodynamical variables, together with the independent time variable. Here the choose for $\mathcal{B}^*$ amounts to choose $(\mathbf{M}, \mathbf{C}, e, \nabla\theta, \boldsymbol{\pi}, \nabla\boldsymbol{\pi})$ as thermodynamical variables, i.e. to set

$$\mathcal{B}^* = Lin(\nu)\oplus Lin(\nu)\oplus\mathbb{R}\oplus\nu\oplus\nu\oplus Lin(\nu) \simeq \hat{B},$$

not forgetting that $\mathbf{M}$ and $\mathbf{C}$ are redundant with respect to $\tilde{\mathcal{B}}$ according to the discussion of the Appendix.

References

Ciancio, V.; Cimmelli, V. A.; Valanis, K. C.: A thermodynamic theory of thermoelastic and viscoanelastic solids with non-Euclidean structure. *J. Non-Equilibrium Thermodyn.*, 26, (2001), 153–166.

Coleman, B. D.; Owen, D. R.: Arch. rat. mech. anal. *A mathematical foundation for thermodynamics*, 54, (1974), 1–104.

De Groot, S. R.; Mazur, P.: *Non-Equilibrium Thermodynamics*. North-Holland P. C., Amsterdam (1962).

Dolfin, M.; Francaviglia, M.; Rogolino, P.: A geometric perspective on irreversible thermodynamics with internal variables. *Journal of Non-Equilib. Thermod.*, 23, (1998a), 250–263.

Dolfin, M.; Francaviglia, M.; Rogolino, P.: *Proc. of "The International Symposium on Trends in Continuum Physics"*, Poznan, Poland, 17-20 August, (1998b).

Dolfin, M.; Francaviglia, M.; Rogolino, P.: A geometric model on the thermodynamics of simple materials. *Periodica Polytechnica - Budapest Serie Mech. Eng.*, 43, (1999).

Eringen, A. C.; Maugin, G. A.: *Electrodynamics of Continua, Foundations and solid media*. Springer-Verlag, New York-etc.. (1989).

Francaviglia, M.; Ciancio, V.; Dolfin, M.: Localization of deformations in finite elastoplasticity. *Technische Mechanik*, 22, (2002), 111–117.

Kittel, C.: *Introduction to Solid State Physics*. John Wiley and Sons, New-York (1966).

Maugin, G. A.: Deformable dielectrics I. Field equations for a dielectric made of several molecular species. *Arch. Mech. (Poland)*, 28, (1976), 676–682.

Maugin, G. A.: Deformable dielectrics II. Voigt's intramolecular force balance in elastic dielectrics. *Arch. Mech. (Poland)*, 29, (1977a), 143–159.

Maugin, G. A.: Deformable dielectrics III. A model of interactions. *Arch. Mech.*, 29, (1977b), 251–258.

Maugin, G. A.: The method of virtual power in continuum mechanics: application to coupled fields (review paper). *Acta. Mech.*, 35, (1980), 1–7.

Maugin, G. A.: *Continuum Mechanics of Electromagnetic Solids*. North Holland Series in Applied Mathematics and Mechanics, North-Holland-Amsterdam (1988).

Maugin, G. A.: Internal variables and dissipative structures. *J. Non-Equilib. Thermodyn.*, 15, (1990), 173–192.

Maugin, G. A.; Pouget, J.: Acoustic equations for one-domain ferroelectric. *J.Acoust. Soc. Am.*, 68, (1980), 575–587.

Müller, I.: *Thermodynamics*. Pitman Advanced Publishing Program, London (1985).

Muschik, W.: Internal variables in non-equilibrium thermodynamics. *J. Non-Equilibrium Thermodynamics*, 15, (1990), 127–137.

Noll, W.: Arch. rat. mech. anal. *A mathematical theory of the mechanical behaviour of continuous media*, 2, (1958), 197–226.

Owen, D. R.: *A first course in the mathematical foundations of thermodynamics*. Springer-Verlag, New York (1984).

Valanis, K. C.: The concept of physical metric in thermodynamics. *Acta Mechanica*, 113, (1995), 169–184.

Verhas, J.: *Thermodynamics and rheology*. Kluwer Avad. Publ., Dordrecht, The Netherlands (1997).

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