Elastic-plastic deformation of a single crystal in a geometrized theory of thermodynamic spaces with internal variables

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Abstract

In this paper the microstructural model of a single crystal based on the use of the local, current and lattice configuration is shortly presented. Our analysis of the model generalizes the study in [15] to non-equilibrium systems. In particular, we consider a reverse Lee decomposition for the deformation gradient and we choose an appropriate state space in which one of the variables, characterizing the internal disarrangement, is given as an internal variable. The dissipation inequality and thermodynamic restrictions are obtained in both Lee decompositions.

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1 Introduction

This paper is concerned with a geometrical framework for thermodynamic spaces already introduced in the papers [1, 2], where we have considered a material element and defined the state space at time t as the set B_t of all state variables which "fit" the configuration of the element at time t. We assume that B_t has the structure of a finite dimensional manifold. The "total state space" is then given by the disjoint union

$$\mathcal{B} = \cup_t \{t\} \times B_t \tag{1.1}$$

with a given natural structure of fibre bundle over the real line $\mathbb{R}$ where time flows [3, 4]. If the instantaneous state space B_t does not vary in time the state space $\mathcal{B}$ reduces to a Cartesian product $\mathbb{R} \times B$. Moreover we consider an abstract space of *processes* [5] which consists of a set Π of functions

$$P_t^i : [0, t] \to \mathcal{G} \tag{1.2}$$

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where $[0, t]$ is any time interval, the space $\mathcal{G}$ 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. Then, a continuous function is defined

$$\rho : \mathbb{R} \times \Pi \to C^0(B_0, B_t) \tag{1.3}$$

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 the real processes occur outside equilibrium. Thermodynamical theories describing transformations induced by processes of this kind are known [6] as *non-equilibrium theories.* They consist in describing the system in such a state of non-equilibrium using the same 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.*

The notion of internal variable is well-known [7] and we shall not comment here about it. We just mention that it was first introduced by considering chemical reactions; the concept was later applied to constitutive equations of dissipative materials such as viscoelastic and viscoplastic ones [8].

Let us now recall that finite elastic and plastic deformations of solids have been analyzed by Lee and co-workers [9, 10] by decomposing the total *deformation gradient* tensor $\mathbf{F}$ into an *elastic deformation* $\mathbf{F}^e$ and a *plastic deformation* $\mathbf{F}^p$ according to the rule:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p.$$

The general theory of elastoplasticity and thermoplasticity is in fact based on the multiplicative decomposition (1) of the deformation gradient. This decomposition of the deformation gradient can be imagined as a result of a local unloading process, which does not take place in reality and which leads to the concept of an *intermediate configuration* [11]. Then the basic idea is to consider three configurations. The first configuration is the initial undisturbed state while the third describes the state after elastic-plastic deformation. If the stress in the final configuration is removed and the temperature is reduced to the uniform initial temperature, the elastic and thermal deformation will be recovered, leaving only permanent plastic deformations which provide the second (intermediate) configuration [12]. The final configuration and the unstressed state are considered to be associated with the state of the body at each instant of time t during the development of plastic flow. The total deformation can be then considered as being obtained through thermoelastic strain from the plastically deformed configuration.

Let us also recall the possibility of reversing the order of the elastic and plastic deformations in the decomposition (1), giving the following reverse decomposition:

$$\mathbf{F} = \mathbf{F}^p \mathbf{F}^e \tag{1.4}$$

This reverse decomposition (1.4) was discussed in [12] (see also [18]), where it was shown that finite elastic and plastic deformations of *isotropic* solids can be analyzed using either decomposition (1) or (1.4). As in general the matrix product is non-commutative, the two decompositions turn out to be different.

We are aware that the reverse decomposition (1.4) is usually considered to be controversial and no stringent physical arguments have yet justified it. Moreover, we believe that the arguments of [12] can be fruitfully extended to cover the much more interesting case of non-isotropic materials, in which the decomposition (1.4), in this case fully non-equivalent to (1), amounts to assume that an elastic displacement is first undergone before the material undergoes a plastic relaxation. These is no reason whatsoever to postulate which one effect happens first, since a reasonable model of elasto-plastic relaxation should in fact be the limit of a practically continuous sequence of elastic slips and plastic relaxations. The choice of (1.4) in a sense corresponds to under which are the effects of an elastic slip which *follows* in time a plastic relaxation happened slightly before. Because of this, considering (1.4) is not, in our opinion, just a curiosity, since it could suggest the possibility of different phenomena.

The aim of this paper is twofold. On one hand we aim to apply the alternative decomposition (1.4) for the model of a single crystal already developed by Asaro in [14], where the "standard" decomposition (1) was considered, and to obtain, also in this case, the corresponding new constitutive laws and the dissipation inequality as well. On the other hand, our analysis will not just reproduce the analysis of [15] for the case (1), as it should, but it will in fact generalize it to the case of thermodynamical non-equilibrium, since (differently from [15]) we shall allow a non zero gradient of temperature. These results, which will be given both for the standard decomposition and the non-canonical reverse one, have a great importance for the understanding of all situations in which the temperature cannot be constant, a case in which non-isotropic materials (e.g. when fractures or plasticity have to be considered) are more appropriately investigated.

The large deformation of inelastic materials involves various microscopic processes such as *slip* over crystallographic planes that interact with each other producing a rather complicated global behavior [16]. In fact, as remarked in [17, 18] by Teodosiu: "*the physical research on plastic and viscoplastic, i.e. crystalline materials, has revealed the existence of an internal mechanical state which is the lattice defect state. The quantities used for the description of this state are called internal quantities*". When talking about plasticity, the most important variable part of the internal state is the *dislocation state*. Indeed, physical research shows that plasticity and viscoplasticity are typical properties of crystalline material, and the defects, like e.g. the dislocations, are the principal factors of some process which can be observed at macroscopic level via the permanent deformations produced. Among the defects of the crystalline structure, the *line defects* are those which produce the plastic permanent deformations and involve changes of the internal mechanical structure during the deformation process [18].

2 The model of a single crystal

Plasticity and viscoplasticity in finite strains are basic effects in the behaviour of single crystals for which the finiteness of strain is essential [19, 21]. The plastic deformation occurs in the form of smooth shearing deformations on certain planes of a crystal (say p_α, with $1 \leq \alpha \leq N$) and in certain permissible directions l_α on each such plane. More generally one side of the crystal slips on a *slip surface* with respect to the other part, along a determined direction, called the *slip direction*; often this surface is a plane called the *slip plane* [18]. The allowed planes and directions constitute the set of *slip systems* of the crystal [20]. The slip in a slip system begins when the shear stress in the slip plane, called the *reduced shear stress*, reaches a critical value. This critical value varies depending on the temperature and on the rate of deformation. Throughout the slip process the material mantains its crystalline structure [18].

Following [17] in a finite deformation theory of elastoplasticity of single crystals we need to take into account that the dislocation passing through a volume element produces an irreversible and permanent change of its shape, even if the mean orientation of the crystalline structure does not change. In the case of non-uniform viscoplastic deformations, the deformations of the volume elements are incompatible with each other, bringing about elastic deformations and *residual stresses*. The stresses produced by the dislocations which remain inside a volume element delay the motion of the dislocations themselves. This leads to the *hardening* of the material observed at a macroscopic level. Even if the elementary slip produced by each dislocation is discontinuous, the plastic deformation and the elastic deformation may be considered to be continuous at macroscopic level due to the high dislocation density [18]. An extensive literature exists concerning the constitutive theory of thermoelastoviscoplastic deformations of the materials with intermediate relaxed configurations and internal state variables (see e.g. [10, 13]).

Several authors have investigated costitutive laws for the elastic-plastic deformation of crystals at finite strain. Usually they considered the case in which the material particles flow through the crystal lattice via dislocation motion whereas the lattice undergoes elastic deformations. Then there are two physically different processes for deforming and reorienting materials, i.e. plastic slip and lattice deformation [14]. In [14, 15] a model of single crystal undergoing single slip on a slip system is described, where the slip system is defined by a pair of orthogonal unit vectors in the reference state. The total deformation and rotation of the crystal is given by the deformation gradient $\mathbf{F}$, which can be written using Lee's decomposition (1), i.e.:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p, \tag{2.1}$$

where $\mathbf{F}^p$, with $det\mathbf{F}^p = 1$, is the deformation due solely to plastic shearing on crystallographic slip systems and $\mathbf{F}^e$ with $\det\mathbf{F}^e \neq 0$ is caused by stretching and rotation of the crystal lattice. The deformation gradient remaining after elastic unloading and upon returning the lattice to its orientation in the reference state is (see [14]):

$$(\mathbf{F}^e)^{-1}\mathbf{F} = \mathbf{F}^p.$$

Unlike $\mathbf{F}$, both tensors $\mathbf{F}^p$ and $\mathbf{F}^e$ are not necessarily gradients of motion; since $\mathbf{F}^p$ and $\mathbf{F}^e$ are invertible, they do still represent in any case deformations of infinitesimal neighborhoods. As we said above, the motion of dislocations is assumed to take place on a prescribed set of slip systems $(\mathbf{s}^\alpha, \mathbf{m}^\alpha)$, where α is an index running in an arbitrary index set denoting its slip plane p_α; each pair is formed by a direction $\mathbf{s}^\alpha$ and a slip-plane normal $\mathbf{m}^\alpha$, where $\mathbf{s}^\alpha$ and $\mathbf{m}^\alpha$ are orthogonal constant vectors in the lattice configuration such that:

$$|\mathbf{s}^\alpha| = |\mathbf{m}^\alpha| = 1, \ \mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0.$$

3 Analysis of the model: earlier results

Let us briefly recall here the ideas and results obtained for this model in [15] on the basis of the decomposition (1) and a few additional hypotheses.

Since the plastic flow occurs in the slip, an evolution of $\mathbf{F}^p$ is expressed by slip rates ν^α on the individual slip through the following ansatz

$$\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p, \tag{3.1}$$

where a matrix $\mathbf{L}^p$ appears defined by

$$\mathbf{L}^p = \sum_\alpha \nu^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha. \tag{3.2}$$

The theory developed in [15] considers together with classical macroforces also microforces represented by stresses ξ^α and internal forces Π^α for each slip system α consistent with a microforce balance; this balance equation is considered with the classical Newtonian balances for momentum [15]. Denoting by $\mathbf{T}_{ref}$ and $\mathbf{b}$ the *stress* and the *body force*, measured respectively per unit area and per unit volume in the reference configuration, the standard force and momentum balances take the following local forms:

$$Div \mathbf{T}_{ref} + \mathbf{b} = 0 \tag{3.3}$$

$$\mathbf{T}_{ref} \mathbf{F}^T = \mathbf{F} \mathbf{T}_{ref}^T, \tag{3.4}$$

where X^T denotes the transpose matrix of a matrix X. If $\mathbf{T}$ is the Cauchy stress tensor then equation (3.4) can be rewritten as

$$\mathbf{T}_{ref} = (det \mathbf{F}) \mathbf{T} \mathbf{F}^{-T}. \tag{3.5}$$

After having introduced the *lattice stress* $\mathbf{S}$ by

$$\mathbf{S} = (det \mathbf{F}^e)(\mathbf{F}^e)^{-1} \mathbf{T} (\mathbf{F}^e)^{-T}$$

the expression

$$\mathbf{S} = (\mathbf{F}^e)^{-1} \mathbf{T}_{ref} (\mathbf{F}^p)^T \tag{3.6}$$

holds and the equation (3.4) turns out to be equivalent with the property of $\mathbf{S}$ being symmetric.

The work of the standard forces is defined in the classical form for any part P of the body by the volume integral

$$W_{stan}(P) = \int_P \mathbf{T}_{ref} \cdot \dot{\mathbf{F}} dv \tag{3.7}$$

where the integrand function is the standard *stress power*. Here and in the sequel a dot means full contraction of tensors; e.g., for rank two tensors one has $\mathbf{A} \cdot \mathbf{B} = A_{ij} B^{ij} = tr(\mathbf{A}^T \mathbf{B})$, where T denotes transposition. The microforces of the system are characterized by microstresses ξ^α, internal microforces Π^α and external microforces μ^α such that the following local balance is satisfied:

$$Div\xi^\alpha - \Pi^\alpha + \mu^\alpha = 0 \tag{3.8}$$

The justification for the independent existence of equation (3.8) can be found in [15], to which we refer the reader for further details.

The microforces Π^α provide a macroscopic description of forces exerted on the dislocations of the α-th plane of the system by dislocations of the other slip systems and by the lattice or other defects; these forces are internal to the material. The microforces μ^α represent forces exerted on dislocations by actions which are external to the body. These microforces perform work together with the atomic disarrangements; the work of the microforces is then given by the volume integral

$$W_{mic}(P) = \sum_\alpha \int_P [\xi^\alpha \cdot \nabla\nu^\alpha + \Pi^\alpha \nu^\alpha] dv, \tag{3.9}$$

where (3.8) together with Stokes' theorem has been used. This expression represents the work of all microforces which are internal to P, i.e. a micropower balance for any part P of the body.

Standard forces and microforces interact internally through a force balance relating the two quantities. Then, the total internal work is given by the sum of two works above, i.e.:

$$W_{stan}(P) + W_{mic}(P) = \int_P [\mathbf{T}_{ref} \cdot \dot{\mathbf{F}} + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \Pi^\alpha \nu^\alpha)] dv. \tag{3.10}$$

Taking the time-derivative of the decomposition (1) and using the ansatz (3.1) and (3.2) yields

$$\dot{\mathbf{F}} = \dot{\mathbf{F}}^e \mathbf{F}^p + \mathbf{F}^e [\sum_\alpha \nu^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha] \mathbf{F}^p. \tag{3.11}$$

Following a sugestion of Gurtin [15] we assume now that the internal work is determined by $\dot{\mathbf{F}}^e$ and ν, rather than by $\dot{\mathbf{F}}$ and ν. This amounts, as in [15], to assume the existence of a lattice stress $\mathbf{T}^e$ conjugate to $\dot{\mathbf{F}}^e$ and an internal microforces π^α conjugate to ν^α. it is then possible to consider the internal work as being expressed by the relation

$$W_{stan}(P) + W_{mic}(P) = \int_P [\mathbf{T}^e \cdot \dot{\mathbf{F}}^e + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \pi^\alpha \nu^\alpha)] dv. \tag{3.12}$$

Since the two relations (3.10) and (3.12) have to coincide for all P and for all choices of $\dot{\mathbf{F}}$, ($\dot{\mathbf{F}}^e$) and ν, the following relation is obtained in [15]:

$$\mathbf{T}_{ref} \cdot \dot{\mathbf{F}} + \sum_\alpha \Pi^\alpha \nu^\alpha = \mathbf{T}^e \cdot \dot{\mathbf{F}}^e + \sum_\alpha \pi^\alpha \nu^\alpha \tag{3.13}$$

In particular, this holds for $\nu = 0$ and in such a case one obtains $\dot{\mathbf{F}} = \dot{\mathbf{F}}^e \mathbf{F}^p$ together with the relation

$$\mathbf{T}^e = \mathbf{T}_{ref}(\mathbf{F}^p)^T. \tag{3.14}$$

Finally, by using (3.6) this last equation is rewritten ([15])

$$\mathbf{T}^e = \mathbf{F}^e\mathbf{S} \tag{3.15}$$

in terms of the lattice stress $\mathbf{S}$. Analogously, for any fixed α, by choosing $\dot{\mathbf{F}} = 0$, and using equation (3.13) with $\nu^\beta = 0$ if $\beta \neq \alpha$ the following relations are deduced in cite:

$$\begin{aligned} \dot{\mathbf{F}}^e &= -\mathbf{F}^e(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\nu^\alpha \\ \Pi^\alpha &= -\mathbf{T}^e \cdot [\mathbf{F}^e(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)] + \pi^\alpha. \end{aligned} \tag{3.16}$$

The physical significance of equations (3.16) is not discussed in [15]. We notice that, according to the general rule $\dot{\mathbf{F}} = \mathbf{L}\mathbf{F}$, equation $(3.16)_1$ amounts to say that for α fixed and $\nu^\beta = 0$ if $\beta \neq \alpha$ the "elastic velocity gradient" $\mathbf{L}^e$ is just the tensor $(-\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\nu^\alpha$, i,e. a virtual elastic gradient of velocity which is proportional to the tensor product of the two parameters which define the α-th slip plane. The second equation $(3.16)_2$ can be then seen as an explicit expression of the difference between macro- and micro-forces as driven by the inner product $\mathbf{T}^e \cdot \mathbf{L}^e$, as one should expect.

4 Analysis of the model in the alternative decomposition

In this section we shall apply the alternative "reverse" decomposition (1.4) for the deformation gradient to the model of a single crystal developed in [14, 15] and already described in the previous sections. We shall see that different relations arise when specifying $\mathbf{F}$ and $\dot{\mathbf{F}}$ and the new results should be compared with those of [15] recalled in section 3. We first adapt and revert the analysis made by Gurtin in [15], using now the lattice configuration for the configurations obtained by locally applying $\mathbf{F}^e$ to the reference increments. In this alternative perspective, $\mathbf{F}^e$ goes from the reference configuration to the lattice configuration while $\mathbf{F}^p$ goes from the lattice configuration to the deformed (or current) one. The main idea consists then in privileging, as far as possible, quantities depending on $\mathbf{F}^p$ rather than quantities depending on $\mathbf{F}^e$.

In the present analysis the evolution equation for the plastic deformation gradient $\mathbf{F}^p$ is preserved, it being still given by eqn.s (3.1) and (3.2). Also the momentum balance, microforce and standard force balances and their works, maintain here the same form expressed, respectively, by (3.4), (3.3), (3.8), (3.7) and (3.9). Since the total internal work is still governed by equations (3.10) and (3.12), the identity (3.13) valid in the original decomposition (1), will be now assumed as an ansatz for the alternative decomposition (1.4), still valid for all tensors $\dot{\mathbf{F}}$ and $\dot{\mathbf{F}}^e$ and for all ν^α.

In full analogy with the to previous analysis, by taking here into account the decomposition (3.4) and by recalling that both $\mathbf{F}^e$ and $\mathbf{F}^p$ are invertible, the tensor $\mathbf{T}_{ref}$ still defined by (3.5) takes now the alternative form

$$\mathbf{T}_{ref} = \mathbf{F}^p\mathbf{Z}(det\mathbf{F}^e)(\mathbf{F}^e)^{-T}, \tag{4.1}$$

where the tensor $\mathbf{Z}$ denotes the "alternative" (or "plastic") lattice stress and is defined by the inverse relation:

$$\mathbf{Z} = (det\mathbf{F}^e)^{-1}[(\mathbf{F}^p)^{-1}\mathbf{T}_{ref}(\mathbf{F}^e)^T]. \tag{4.2}$$

Notice that $\mathbf{F}^p$ plays in $\mathbf{Z}$ a role similar to the role played by $\mathbf{F}^e$ in the tensor $\mathbf{S}$ given by (3.6). We compute now the total time derivative of the deformation gradient assuming that it is now defined by equation (1.4). We obtain then from (3.1) and (3.2) the alternative expression

$$\dot{\mathbf{F}} = (\sum_\alpha \nu_\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\mathbf{F}^p\mathbf{F}^e + \mathbf{F}^p\dot{\mathbf{F}}^e, \tag{4.3}$$

which in our analysis replaces (3.11). As before, with the choice $\nu = 0$ the equality (4.3) reduces to $\dot{\mathbf{F}} = \mathbf{F}^p\dot{\mathbf{F}}^e$ and the ansatz (3.13) leads to the expression

$$\mathbf{T}^e = (\mathbf{F}^p)^T\mathbf{T}_{ref}. \tag{4.4}$$

Then, using again the definition of $\mathbf{T}_{ref}$ as given by (4.1) we obtain the alternative form of $\mathbf{T}^e$ as a function of the "plastic" lattice stress $\mathbf{Z}$

$$\mathbf{T}^e = (\mathbf{F}^p)^T\mathbf{F}^p\mathbf{Z}(det\mathbf{F}^e)(\mathbf{F}^e)^{-T} \tag{4.5}$$

Taking finally $\dot{\mathbf{F}} = 0$ for any fixed α one obtains the alternative relations:

$$\begin{aligned} \dot{\mathbf{F}}^e &= -(\mathbf{F}^p)^{-1}\Big[\sum_\alpha(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\mathbf{F}^p\mathbf{F}^e\Big] \\ \Pi^\alpha &= -\mathbf{T}^e \cdot \Big[(\mathbf{F}^p)^{-1}\sum_\alpha(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\mathbf{F}^p\mathbf{F}^e\Big] + \pi^\alpha. \end{aligned} \tag{4.6}$$

Comparing these results with those of the last section, we see that the expressions (4.4), (4.5) and (4.6) replace, respectively, the relations (3.14), (3.15) and (3.16). Their physical significance is analogous, with obvious changes, to the meaning of conditions (3.16) as we already discussed at the end of Section 3.

5 Entropy analysis and thermodynamical restrictions

In this last section we perform the analysis of the second law of thermodynamics for both models of Section 3 and 4. Results are essentially new also for the original model of [15].

Let us then consider a slip system which undergoes irreversible processes far from equilibrium and let us suppose it be characterized by a state space given by $(\mathbf{F}^e, \xi^\alpha, \theta, \nabla\theta)$, where θ represents the temperature scalar field of the slip. As we said before, the scalar internal variables ξ^α characterize the state of internal rearrangement, so that we can follow the internal variable formulation for entropy developed in our earlier papers [2]. Since the total internal work gives a contribution to the time variation of the internal energy u of the system we have the energy balance [15]

$$\int_P \dot{u}\, dv = W_{stan} + W_{micr} - \int_P (div\, \mathbf{q})\, dv, \tag{5.1}$$

where $\mathbf{q}$ is the heat flux vector.
Let us then express the second law through the classical Clausius-Duhem inequality [22]

$$\dot{S} + div \frac{\mathbf{q}}{\theta} \geq 0, \tag{5.2}$$

where the term S denote the entropy function. By introducing the *free energy*,

$$\Psi = u - \theta S$$

and calculating the total time derivative of Ψ eqn. (5.2) becomes

$$-(\dot{\Psi} + \dot{\theta} S) + \dot{\mathbf{T}}^e \cdot \mathbf{F}^e + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \pi^\alpha \nu^\alpha) - \frac{\mathbf{q}}{\theta} \cdot \nabla\theta \geq 0, \tag{5.3}$$

where (3.12) has been used. Since the *equipresence principle* forces us to postulate the constitutive equation for Ψ, as well as all other constitutive quantities, in the following form

$$\Psi = \Psi^*(\mathbf{F}^e, \xi^\alpha, \theta, \nabla\theta),$$

the total time derivative $\dot{\Psi}$ can be generally expressed by

$$\dot{\Psi} = \frac{\partial\Psi^*}{\partial\mathbf{F}^e}\dot{\mathbf{F}}^e + \frac{\partial\Psi^*}{\partial\xi^\beta}\dot{\xi}^\beta + \frac{\partial\Psi^*}{\partial\theta}\dot{\theta} + \frac{\partial\Psi^*}{\partial\nabla\theta}(\nabla\theta)^{\cdot}, \tag{5.4}$$

where the first addendum represents the change in the free energy due to stretching of the reference state, the second addendum represents changes induced by slip, the third one considers change of temperature and the last one is due to non-uniform temperature.

By substituting equations (5.1), (5.4), (3.7) and (3.9) into (5.3), we have now the inequality

$$\begin{aligned} &\Big(-\frac{\partial\Psi^*}{\partial\mathbf{F}^e} + \mathbf{T}^e\Big)\dot{\mathbf{F}}^e - \sum_\beta \frac{\partial\Psi^*}{\partial\xi^\beta}\dot{\xi}^\beta + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \pi^\alpha\nu^\alpha) + \\ &-\Big(\frac{\partial\Psi^*}{\partial\theta} + S\Big)\dot{\theta} + \frac{\partial\Psi^*}{\partial\nabla\theta}\nabla\dot{\theta} - \frac{\mathbf{q}}{\theta}\nabla\theta \geq 0. \end{aligned} \tag{5.5}$$

By applying the usual procedure to restrict constitutive equations [7, 22] the following relations finally occur:

$$\frac{\partial\Psi^*}{\partial\mathbf{F}^e} = \mathbf{T}^e \tag{5.6}$$

$$\frac{\partial\Psi^*}{\partial\nabla\theta} = 0 \tag{5.7}$$

$$\frac{\partial\Psi^*}{\partial\theta} = -S, \tag{5.8}$$

which, because of our discussion, cover both cases of decompositions (1) and (1.4). Obviously in the case (1) already considered in [15] the tensor $\mathbf{T}^e$ is expressed by means of $\mathbf{S}$ as in (3.15); while in the case of (1.4) the tensor $\mathbf{T}^e$ is expressed in terms of $\mathbf{Z}$ by means of (4.5). We remark that eqn. (5.6) coincides only formally with eqn. $\mathbf{S} = \frac{\partial \Psi^*(s)}{\partial E^e}$ derived in [15] by considering a mechanical version of second law relating the temporal change in free energy to the rates at which work is performed and to energy dissipated. In this equation the term $\mathbf{E}^e = \frac{1}{2}[(\mathbf{F}^e)^T\mathbf{F}^e - \mathbf{1}]$ is referred to lattice strain and $s = (\mathbf{E}^e, \mathbf{F}^p, \sigma)$ denotes the state, i.e. the set of independent variables, where σ is treated as an internal state variable that represents the slip resistences, i.e. dissipative internal forces that oppose to slip.

In our analysis we introduce the temperature not requiring it to be constant and a gradient $\nabla\theta$ enters the state variables. Let us finally notice that using the thermodynamical restrictions (5.6), (5.7) and (5.8) the inequality (5.5) can be reduced to the following residual dissipation inequality

$$-\sum_\beta \frac{\partial \Psi^*}{\partial \xi^\beta}\dot{\xi}^\beta + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \pi^\alpha \nu^\alpha) - \frac{\mathbf{q}}{\theta}\nabla\theta \geq 0, \tag{5.9}$$

in which we involve the following two components:

$$\Phi_{int} \equiv -\sum_\beta \frac{\partial \Psi^*}{\partial \xi^\beta}\dot{\xi}^\beta + \sum_\alpha (\xi^\alpha \cdot \nabla\nu^\alpha + \pi^\alpha \nu^\alpha) \tag{5.10}$$

$$\Phi_{th} \equiv -\frac{\mathbf{q}}{\theta}\nabla\theta, \tag{5.11}$$

which correspond to the intrinsic and thermal dissipations respectively, as introduced in [22]. Equation (5.9) imposes that the sum of Φ_{int} and Φ_{th} is positive, being zero only for reversible processes. We remark (see [23]) that stronger conditions can be imposed, in order to have

$$\Phi_{int} \geq 0, \quad \Phi_{th} \geq 0 \tag{5.12}$$

separately. For $\nu = 0$, by $(5.12)_1$, it follows that the intrinsic dissipation, for the arbitrarity of the vectors $\dot{\xi}^\beta$, has to be positive and should force the rates of internal rearrangement occurring during a process to be such that the free energy decreases if $\mathbf{F}^e$ and $\nabla\theta$ are held fixed. To the same conclusion was also led Rice in [20], who considered however as thermodynamic state variables the stress, the temperature and a set of scalar internal variables and in which $\nabla\theta = 0$.

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