

Thermodynamics of Local State : Overall Aspects and Micromechanics Based Constitutive Relations

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The thermodynamics of irreversible processes, based on a set of internal state variables, is revisited, paying attention on two complementary aspects :

- The Generalized Standard Models are shown to introduce too stiff constraints, both for kinematic hardening and for damage modellings. A slightly less restrictive approach is then considered, based on several independent potentials and several independent multipliers ;

- The micro-macro approach of elastoplasticity is formulated through the Transformation Field Analysis of Dvorak and the use of a correction method. Moreover, based on previous works of Suquet and Nguyen, the approach is generalized with energy considerations, incorporating continuous fields of eigenstrains.

1 Introduction

Thermodynamics of irreversible processes represents an excellent framework for the development of constitutive and damage equations. In particular, using one of its versions based on the notion of local state and internal state variables Germain (1974), Germain (1973), induces sufficient constraints against a too large set of possibilities.

Such a framework has been extensively used during the past thirty years, in many different contexts Sidoroff (1975), Chaboche (1978), Krajcinovic and Fonseka (1981), Ju (1989), Hansen and Schreyer (1994), including plasticity and viscoplasticity of metals, creep, inelastic behaviour of geomaterials (soils, rocks, concrete, salt,...), Continuum Damage Mechanics, etc. Many improvements and more rigorous choices in the inelastic and damage constitutive equations of representative materials were obtained within this framework.

The purpose of the present paper is twofold :

- review some of the properties of the thermodynamics with internal variables, especially the notion of Generalised Standard Models (GSM) Halphen and Nguyen (1975), together with some too strict limitations of this formulation. Then present a more recent extension, called here the "*pseudo-standard approach*", that offers slightly less restrictive rules ;
- discuss some of the properties of constitutive equations deduced from macro-homogenisation tools in the light of thermodynamic aspects. In this context we consider the *Transformation Field Analysis* (TFA) method, developed by Dvorak and co-workers Dvorak and Benveniste (1992), Dvorak (1992). This approach, mainly useful for composite systems, is revisited in energy terms (state potential and dissipation), based on discussions previously given by Suquet (1982) and Nguyen (1988), in an insufficiently known context.

2 The Continuum Thermodynamic Framework : Standard and Less Standard Approaches

2.1 General Requirements

We follow the classical presentation and general assumptions (see for instance Germain (1973)), considering only quasi-static movements and the small perturbation theory. The hypothesis of "local state" implies that the present internal state of a material point in a structure (and its surrounding Representative Volume Element, RVE) is independent of the corresponding state at the neighbouring material points.

In fact the notion of a RVE is more or less subjective for real materials and actual structural situations. We have to assume that the microstructural lengthscale (the average size of the microstructural elements) is negligible compared with the RVE size and, at the same time, that this RVE is negligibly small against the structural size (or the wavelength of the global stress/strain fields on the structure). In the present discussion we deliberately stay in the context of classical continua, without any of the "material lengthscales" that are involved in Generalised Continuum Mechanics.

The small perturbation assumption allows us to write additively the decomposition of total strain $\underline{\varepsilon}$ into :

$$\underline{\varepsilon} = \underline{\varepsilon}^{e\theta} + \underline{\varepsilon}^p = \underline{\varepsilon}^e + \underline{\varepsilon}^\theta + \underline{\varepsilon}^p \quad (1)$$

where $\underline{\varepsilon}^{e\theta}$, $\underline{\varepsilon}^\theta$ and $\underline{\varepsilon}^p$ are respectively the thermoelastic strain (reversible part of the strain), the thermal expansion ($\underline{\varepsilon}^\theta = \alpha \theta = \alpha (T - T_o)$) and the plastic or viscoplastic strain (the irreversible part). The present state of the material is characterized by the knowledge of observable variables, the total strain and temperature T , and by a set of internal state variables ($\underline{\varepsilon}^p$, a_j) associated with plasticity, viscoplasticity, the corresponding hardening processes, aging effects, etc, as well as damage processes and related effects. These internal state variables store the effect of the whole history of observable variables, that appear in the hereditary theories. The plastic strain itself $\underline{\varepsilon}^p$ is considered as one of these internal variables. We assume the existence of a thermodynamic state potential, as sufficient to describe all the reversible processes (here we will use the Helmholtz free energy). This depends on all the state variables : $\psi = \psi(\underline{\varepsilon}, \underline{\varepsilon}^p, T, a_j)$. The First and Second Principles of thermodynamics are used to derive the laws of thermoelasticity, following a classical treatment Coleman and Gurtin (1967) :

$$\underline{\sigma} = \frac{\partial \psi}{\partial \underline{\varepsilon}} = \frac{\partial \psi}{\partial \underline{\varepsilon}^e} \quad \mathcal{S} = -\frac{\partial \psi}{\partial T} \quad A_j = \frac{\partial \psi}{\partial a_j} \quad \underline{\sigma}^p = -\frac{\partial \psi}{\partial \underline{\varepsilon}^p} \quad (2)$$

in which $\underline{\sigma}$ is the stress tensor, \mathcal{S} the entropy, A_j the thermodynamic forces associated to the internal variables a_j , and $\underline{\sigma}^p$ the associated force to $\underline{\varepsilon}^p$. The Second principle now expresses, after separating the dissipation into the intrinsic dissipation $\dot{\Phi}_p$ and the thermal dissipation $\dot{\Phi}_{th}$, the two inequalities being assumed to be fulfilled independently :

$$\dot{\Phi}_p = \underline{\sigma}^p : \dot{\underline{\varepsilon}}^p - A_j \dot{a}_j \geq 0 \quad \dot{\Phi}_{th} = -\frac{1}{T} \underline{\mathbf{q}} \cdot \underline{\nabla} T \geq 0 \quad (3)$$

Remark : Here $\underline{\sigma}^p$ is the force conjugate to the plastic strain : it will often be considered as identical to the stress tensor itself. The following example, for Prager's model, illustrates two equivalent possibilities. Let's start with the free energy expressed as :

$$\psi = \psi_e(\underline{\varepsilon}^e) + \psi_p(\underline{\varepsilon}^p) = \frac{1}{2} (\underline{\varepsilon} - \underline{\varepsilon}^p) : \underline{\mathbb{L}} : (\underline{\varepsilon} - \underline{\varepsilon}^p) + \frac{1}{2} \underline{\varepsilon}^p : \underline{\mathbb{C}} : \underline{\varepsilon}^p \quad (4)$$

assuming isothermal conditions and $\underline{\varepsilon}^\theta = 0$. We immediately obtain $\underline{\sigma}^p = \underline{\sigma} - \underline{\mathbb{C}} : \underline{\varepsilon}^p$ and the intrinsic dissipation is $\dot{\Phi}_p = (\underline{\sigma} - \underline{\mathbb{C}} : \underline{\varepsilon}^p) : \dot{\underline{\varepsilon}}^p$. Assuming now ψ_p as depending on an internal variable α , also a second rank tensor that will describe kinematic hardening, we will have $\underline{\sigma}^p \equiv \underline{\sigma}$ and the dissipation $\dot{\Phi}_p = \underline{\sigma} : \dot{\underline{\varepsilon}}^p - \alpha : \underline{\mathbb{C}} : \dot{\alpha}$, where $\underline{\mathbb{X}} = \underline{\mathbb{C}} : \alpha$ can be considered as the back stress. The two cases coincide if we assume linear kinematic hardening in the evolution equation for α , that is $\dot{\alpha} = \dot{\underline{\varepsilon}}^p$. In what follows, we will consider only the second form.

2.2 Generalized Standard Models (GSM)

In the rate independent formulation, if a criterion is assumed concerning physically admissible forces $f(\boldsymbol{\sigma}, A_j)$, corresponding to the elastic domain, the standard material hypothesis consists in considering the normality law for the plastic strain evolution (Hill's maximum dissipation principle) :

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda} \frac{\partial f}{\partial \boldsymbol{\sigma}}, \quad \dot{\lambda} \geq 0, \quad f \leq 0, \quad \dot{\lambda} f = 0 \quad (5)$$

The extension of the normality rule to the evolution equations of other internal variables (in the generalised space of all the conjugate forces) corresponds to the GSM assumption Halphen and Nguyen (1975) :

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda} \frac{\partial f}{\partial \boldsymbol{\sigma}} \quad \dot{a}_j = \dot{\lambda} \frac{\partial f}{\partial A_j} \quad (6)$$

Such a GSM for the rate independent situation of classical plasticity can be generalized both for more complex plasticity rules or for viscoplastic ones, by assuming the existence of a pseudo-potential of dissipations in the space of rate of dissipative variables Germain (1973), Germain et al. (1983) : $\phi = \phi(\dot{\boldsymbol{\varepsilon}}^p, \dot{a}_j; \boldsymbol{\varepsilon}^e, a_j)$. ϕ is supposed to be positive and convex in its main arguments and is assumed to contain origin (that is $\phi(0, 0; \boldsymbol{\varepsilon}^e, a_j) = 0$) for all $\boldsymbol{\varepsilon}^e, a_j$. The state variables $\boldsymbol{\varepsilon}^e$ and a_j , as well as temperature T , act as parameters. The thermodynamic conjugate forces are obtained as :

$$\boldsymbol{\sigma} = \frac{\partial \phi}{\partial \dot{\boldsymbol{\varepsilon}}^p} \quad A_j = \frac{\partial \phi}{\partial \dot{a}_j} \quad (7)$$

Applying to ϕ the Legendre-Fenchel transform, defined by $\phi^*(A) = \min_{\dot{a}} [A \dot{a} - \phi(\dot{a})]$, we obtain the complementary dissipative potential ϕ^* in the generalized space of thermodynamic forces. Equations (7) are then replaced by :

$$\dot{\boldsymbol{\varepsilon}}^p = \frac{\partial \phi^*}{\partial \boldsymbol{\sigma}} \quad \dot{a}_j = -\frac{\partial \phi^*}{\partial A_j} \quad (8)$$

Such a generalized normality confers interesting properties to the constitutive equations. In particular, the second principle is automatically satisfied provided the positiveness and convexity of ϕ^* . Using also $\phi^*(0, 0) = 0$, the intrinsic dissipation (3-a) rewrites as :

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - A_j \dot{a}_j = \boldsymbol{\sigma} : \frac{\partial \phi^*}{\partial \boldsymbol{\sigma}} + A_j \frac{\partial \phi^*}{\partial A_j} \geq \phi^* \geq 0 \quad (9)$$

2.3 Some Important Restrictions

The GSM approach is very attractive but presents some limitations, in the sense of too strict restrictions. This point has been discussed several times in the past Chaboche (1997), Chaboche (1999), and we recall here the problem associated with non linear kinematic hardening. The simple Armstrong-Frederick format, with a "dynamic recovery" term, is used in many constitutive models for cyclic plasticity or cyclic viscoplasticity (see Chaboche (1989).

In the rate independent case, the solution is to consider the indicatrice function F of the convex pseudo-potential of dissipations to be of a non associated form (in the generalized space),

$$F = f + \frac{1}{2} \mathbf{X} : \mathbf{Q} : \mathbf{X} \quad (10)$$

not identical with the function f that describes the elastic domain. If we assume \mathbf{X} to be the back stress we can choose f of the simplest form (neglecting isotropic hardening) :

$$f = \|\boldsymbol{\sigma} - \mathbf{X}\|_H - k = \sqrt{(\boldsymbol{\sigma} - \mathbf{X}) : \mathbf{H} : (\boldsymbol{\sigma} - \mathbf{X})} - k \quad (11)$$

Using the generalized normality rule leads to :

$$\dot{\xi}^p = \dot{\lambda} \frac{\partial F}{\partial \sigma} \quad \dot{\alpha} = -\frac{\partial F}{\partial \underline{\mathbf{X}}} = \dot{\xi}^p - \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{X}}} \dot{p} \quad (12)$$

with $\underline{\underline{\mathbf{X}}} = \underline{\underline{\mathbf{N}}} : \alpha$, where $\underline{\underline{\mathbf{N}}}$, $\underline{\underline{\mathbf{H}}}$ and $\underline{\underline{\mathbf{Q}}}$ are two fourth rank positive definite tensors. We then recover exactly the anisotropic generalization of the Armstrong-Frederick rule Nouailhas (1990). However, in the viscoplastic case (from which the rate independent one should be the limit) we usually have the potential form (8-a) (without multiplier $\dot{\lambda}$ in (12-a)). The way used in Chaboche (1983), Germain et al. (1983) (see also Lemaître and Chaboche (1985)) was to use a viscoplastic potential of the form :

$$\phi_p^* = \frac{D}{n+1} \left\langle \frac{F}{D} \right\rangle^{n+1} \quad F = f + \frac{1}{2} \underline{\underline{\mathbf{X}}} : \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{X}}} - \frac{1}{2} \alpha : \underline{\underline{\mathbf{N}}} : \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{N}}} : \alpha \quad (13)$$

in which α is considered as a parameter. In that case we still obtain :

$$\dot{\xi}^p = \frac{\partial \phi_p^*}{\partial \sigma} = \dot{p} \underline{\underline{\mathbf{n}}} \quad \text{with} \quad \underline{\underline{\mathbf{n}}} = \frac{\underline{\underline{\mathbf{H}}} : (\sigma - \underline{\underline{\mathbf{X}}})}{\|\sigma - \underline{\underline{\mathbf{X}}}\|_H} \quad (14)$$

$$\dot{\alpha} = -\frac{\partial \phi_p^*}{\partial \underline{\underline{\mathbf{X}}}} = \dot{\xi}^p - \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{X}}} \dot{p} \quad (15)$$

Provided the equality $\underline{\underline{\mathbf{X}}} = \underline{\underline{\mathbf{N}}} : \alpha$ can be reused in (13-b), leading continuously to $F \equiv f$, we recover the normal viscoplastic rule with

$$\dot{p} = \left\langle \frac{F}{D} \right\rangle^n = \left\langle \frac{f}{D} \right\rangle^n \quad (16)$$

However such a treatment appears as quite artificial. To some extent it obeys GSM (using state variables as parameters Germain et al. (1983)), but was not considered as GSM by Nguyen (1988)

The choice made by Ladevèze since 1992 Ladevèze (1992), within a purely GSM framework, consists in retaining (13-b) in the viscoplastic case, with ϕ_p as the potential. It produces the expected NLK hardening rule (15) but to the price of a non vanishing extra term in the expression for the true elastic domain :

$$F = f + \frac{1}{2} \underline{\underline{\mathbf{X}}} : \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{X}}} = \|\sigma - \underline{\underline{\mathbf{X}}}\|_H - k^* \leq 0 \quad (17)$$

in which the true elastic limit writes : $k^* = k - \frac{1}{2} \underline{\underline{\mathbf{X}}} : \underline{\underline{\mathbf{Q}}} : \underline{\underline{\mathbf{X}}}$. Such a coupling term between the size of the elastic domain and the back stress induces a significant shortcoming, k^* in (17) must be restricted to always be positive, for obvious reasons. It follows that k , the initial size around $\underline{\underline{\mathbf{X}}} = 0$, must be chosen as very large. If it is not sufficiently large, we will encounter the following shortcomings for significant strains (and high levels of the back stress) : the vanishing of the size of elastic domain, a discontinuity in the tangent stiffness and the non conformity with the GSM Chaboche (1997), Chaboche (1999).

Other limitations of the GSM are related with the Continuum Damage Mechanics models, where we take into account the damage effect on both the elastic behavior and the inelastic one. A thermodynamics based approach naturally involves the conjugate force associated with damage Chaboche (1977) :

$$\dot{d}_k = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial y_k} \quad (18)$$

where we assume a family of damage variables d_k (scalars or tensors). In fact, the use of the GSM approach in that context for the damage growth equations is too restrictive for mainly two reasons :

- for plasticity/viscoplasticity/damage couplings it forces the one-to-one association between the plastic strain evolution and the damage growth, even if different thresholds can be used as in Lemaître's models Lemaître (1985). This can be considered as incorrect for brittle like damage, for example in the creep of metals

(where the accumulated macroscopic strain can be negligible before the complete rupture), or in the damage mechanics of composites ;

- the role of the y_k variables in the dissipation potential does not allow sufficient degrees of freedom for the damage rate equations under multiaxial conditions. In other words there is a too strict association between the damage effect on the elastic behavior and the further damage evolution. Such a strict association has been criticized several times from micromechanics arguments Kachanov (1994).

2.4 A Quasi Standard Model

In order to eliminate the above limitations, we push the idea of a pseudo standard approach in which, instead of one pseudo-potential of dissipation (and an unique scalar multiplier) we could use several pseudo-potentials, defined independently, and several multipliers, defined independently. Each set of potential/multiplier is associated with a particular kind of phenomenon, for example plasticity and associated hardening, static recovery or aging (time effects), damage processes, etc.

The considered formulation then represents a generalization of the classical formalism of plasticity with multiple criteria Mandel (1964) and was already implicitly used in a certain number of works Benallal (1989), Hansen and Schreyer (1992), Zhu and Cescotto (1995). We therefore define three independent potentials, expressed in the space of conjugate forces :

- Ω_p , associated with the plastic flow and the instantaneous hardening processes is assumed to depend on σ and on the hardening forces A_j ;
- Ω_s , associated with the slow (static) microstructural evolution, such as static recovery and aging effects, which is depending essentially on the hardening forces A_j ;
- Ω_d , associated with the damage evolution. This potential is depending on the damage conjugate forces y_k .

Each of these potentials can also depend on the state variables themselves, ε^e , a_j , d_k and T , acting as parameters. In practice we essentially need temperature (for all the thermally activated effects) and the damage variables, for coupling effects on viscoplasticity/hardening evolutions.

The main hypothesis of the proposed Quasi Standard Model is to express the generalized normality rule in the following form :

$$\dot{\varepsilon}^p = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial \sigma} + \dot{\lambda}_s \frac{\partial \Omega_s}{\partial \sigma} + \dot{\lambda}_d \frac{\partial \Omega_d}{\partial \sigma} \quad (19)$$

$$-\dot{a}_j = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial A_j} + \dot{\lambda}_s \frac{\partial \Omega_s}{\partial A_j} + \dot{\lambda}_d \frac{\partial \Omega_d}{\partial A_j} \quad (20)$$

$$\dot{d}_k = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial y_k} + \dot{\lambda}_s \frac{\partial \Omega_s}{\partial y_k} + \dot{\lambda}_d \frac{\partial \Omega_d}{\partial y_k} \quad (21)$$

Of course, with the dependencies considered in the three potentials, certain derivatives vanish, and we obtain :

$$\dot{\varepsilon}^p = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial \sigma} \quad -\dot{a}_j = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial A_j} + \dot{\lambda}_s \frac{\partial \Omega_s}{\partial A_j} \quad \dot{d}_k = \dot{\lambda}_d \frac{\partial \Omega_d}{\partial y_k} \quad (22)$$

The three multipliers $\dot{\lambda}_p$, $\dot{\lambda}_s$, $\dot{\lambda}_d$ are defined freely in terms of all variables, state variables or conjugate forces. In fact, for viscoplasticity, we can take for $\dot{\lambda}_p$ a scalar function of the viscous stress given by the distance f from the current stress state to the elastic domain, in the form of a power function, for example. The simplest definition for $\dot{\lambda}_s$ is to choose a constant value of 1 with the correct units. The choice of $\dot{\lambda}_d$ is not discussed here.

In order to recover the classical formulation of viscoplasticity with Armstrong-Frederick type of kinematic hardening, we chose the particular form :

$$\Omega_p = f + \frac{1}{2} \underline{\mathbf{X}} : \underline{\mathbf{Q}} : \underline{\mathbf{X}} \quad \dot{\lambda}_p = \left\langle \frac{F}{D} \right\rangle^n \quad (23)$$

where $f \leq 0$ defines the elastic domain by (11). Using the above normality rule (eqs (22-a) and (22-b) immediately leads to :

$$\dot{\xi}^p = \dot{\lambda}_p \frac{\partial \Omega_p}{\partial \underline{\sigma}} = \dot{p} \frac{\underline{\mathbf{H}} : (\underline{\sigma} - \underline{\mathbf{X}})}{\|\underline{\sigma} - \underline{\mathbf{X}}\|_H} \quad \dot{\underline{\sigma}} = -\dot{\lambda}_p \frac{\partial \Omega_p}{\partial \underline{\mathbf{X}}} = \dot{\xi}^p - \underline{\mathbf{Q}} : \underline{\mathbf{X}} \dot{p} \quad (24)$$

Contrary to the pure GSM we have the non modified elastic domain, playing role directly in the viscoplastic strain rate. The formulation easily degenerates to the rate independent plasticity format ($f \leq 0$, $D \rightarrow 0$) with $\dot{\lambda}_p$ obtained from the consistency condition $\dot{f} = 0$.

The use of the present Quasi Standard Model was discussed also in the context of CDM Chaboche (1999), and for the modelling of time hardening / aging effects Chaboche et al. (1995), Chaboche (1996).

3 Macrohomogenization Methods

In this section we consider the scale transition methods, between the microscale (or local scale) and the macroscale (or overall scale). Each material point at the microscale, referred as x , has its own surrounding treated as an elementary volume of Continuum Mechanics. The Representative Volume Element (RVE) of the macroscale is constituted of the assemblage (aggregation) of all elementary volumes of the microscale, taking into account on differences in phases, compositions, local orientations, shape of inclusions, etc. It is this RVE that has to be considered in the analysis of components or structures.

We will discuss the transfer of continuum modellings at the microscale to the corresponding informations at the macroscale, through macrohomogenization methods, considering first the stress-strain relations, in thermoelastic / thermoplastic context for a fixed inelastic state, then the energy aspects. We assume small strains and cracks, voids or other displacement discontinuities are not considered. For the notations at the microscale, we continue to use the previous ones of section 2 ($\underline{\xi}$, $\underline{\xi}^p$, $\underline{\xi}^\theta$, $\underline{\sigma}$ for the strain and stress tensors) and the following notations for the corresponding overall quantities : $\underline{\mathbf{E}}$, $\underline{\mathbf{E}}^p$, $\underline{\mathbf{E}}^\theta$, $\underline{\Sigma}$. The local elastic stiffness is denoted $\underline{\mathbb{L}}$ and α is the local thermal expansion coefficient, though $\underline{\bar{\mathbb{L}}}$ and $\bar{\alpha}$ denote the corresponding overall quantities for the RVE. Moreover, we use the following averaging notations :

$$\bar{\rho} = \langle \rho \rangle = \frac{1}{V} \int_V \rho(x) dx \quad \rho_s = \langle \rho \rangle_s = \frac{1}{V_s} \int_{V_s} \rho(x) dx \quad (25)$$

$\bar{\rho}$ represents the average of ρ over the whole RVE volume V , though ρ_s is the average over a subvolume V_s . We denotes the volume fraction $c_s = V_s/V$, so that $\bar{\rho}$ is also $\sum_s c_s \rho_s$. In addition, we cancel everywhere the notations "·" and "·" corresponding to contracted tensorial products.

3.1 Macrohomogenization by TFA

Here, we restrict ourselves to the application and improvement of a method proposed initially by Laws (1973), Willis (1981), Dvorak (1990), Bahei-El-Din (1992). The most elaborated version, called *Transformation Field Analysis* (TFA) Dvorak and Benveniste (1992), incorporates in the same framework thermoelasticity, plasticity, viscoplasticity Dvorak (1992), or even piezo-electricity couplings Benveniste (1993). We like to use this approach, that defines very clearly all the localization operators, concentration tensors and transformation influence functions. For thermo-elastoplastic behaviours, the method uses the linear elastic localization rule and it is pushed together with the notion of piecewise uniform fields, in such a manner that it appears valid only for piecewise uniform eigenstrains. In fact, as shown earlier (see Suquet (1982), Nguyen (1988)), the same formalism can be used for the limit case of continuous fields.

3.1.1 The Elastic Macrohomogenization

We begin by the expression for the local elastic constitutive equations, assuming an uniform elastic stiffness $\underline{\underline{\mathbf{L}}}_r$ over each sub-volume V_r . The local stresses $\underline{\underline{\boldsymbol{\sigma}}}_r(x)$ and strains $\underline{\underline{\boldsymbol{\varepsilon}}}_r(x)$, i.e. quantities at point x in the subvolume V_r , relate by :

$$\underline{\underline{\boldsymbol{\sigma}}}_r(x) = \underline{\underline{\mathbf{L}}}_r \underline{\underline{\boldsymbol{\varepsilon}}}_r(x) \quad \underline{\underline{\boldsymbol{\varepsilon}}}_r(x) = \underline{\underline{\mathbf{L}}}_r^{-1} \underline{\underline{\boldsymbol{\sigma}}}_r(x) \quad (26)$$

At the macroscale, the overall (uniform) strain $\underline{\underline{\mathbf{E}}}$ and stress $\underline{\underline{\boldsymbol{\Sigma}}}$ also relate by :

$$\underline{\underline{\boldsymbol{\Sigma}}} = \underline{\underline{\bar{\mathbf{L}}}} \underline{\underline{\mathbf{E}}} \quad \underline{\underline{\mathbf{E}}} = \underline{\underline{\bar{\mathbf{L}}}}^{-1} \underline{\underline{\boldsymbol{\Sigma}}} \quad (27)$$

In the case of pure elasticity, the local strain and stress fields are connected to the overall ones by the mechanical concentration factors (fourth rank tensors) $\underline{\underline{\mathbf{A}}}_r(x)$ and $\underline{\underline{\mathbf{B}}}_r(x)$:

$$\underline{\underline{\boldsymbol{\varepsilon}}}_r(x) = \underline{\underline{\mathbf{A}}}_r(x) \underline{\underline{\mathbf{E}}} \quad \underline{\underline{\boldsymbol{\sigma}}}_r(x) = \underline{\underline{\mathbf{B}}}_r(x) \underline{\underline{\boldsymbol{\Sigma}}} \quad (28)$$

Let us note immediately the relationship between $\underline{\underline{\mathbf{A}}}_r(x)$ and $\underline{\underline{\mathbf{B}}}_r(x)$ that follows by combining (26), (27) and (28) :

$$\underline{\underline{\mathbf{L}}}_r \underline{\underline{\mathbf{A}}}_r(x) = \underline{\underline{\mathbf{B}}}_r(x) \underline{\underline{\bar{\mathbf{L}}}} \quad (29)$$

Moreover, we immediately obtain the classical relation that defines the overall stiffness tensor :

$$\underline{\underline{\bar{\mathbf{L}}}} = \langle \underline{\underline{\mathbf{L}}}_r \underline{\underline{\mathbf{A}}}_r \rangle = \frac{1}{V} \sum_r \int_{V_r} \underline{\underline{\mathbf{L}}}_r \underline{\underline{\mathbf{A}}}_r(x) dx = \sum_r c_r \underline{\underline{\mathbf{L}}}_r \underline{\underline{\mathbf{A}}}_r \quad (30)$$

Let us note also the relations between local and overall stress and strain :

$$\underline{\underline{\boldsymbol{\Sigma}}} = \underline{\underline{\bar{\boldsymbol{\sigma}}}} = \langle \underline{\underline{\boldsymbol{\sigma}}} \rangle = \sum_r c_r \underline{\underline{\boldsymbol{\sigma}}}_r \quad \underline{\underline{\mathbf{E}}} = \underline{\underline{\bar{\boldsymbol{\varepsilon}}}} = \langle \underline{\underline{\boldsymbol{\varepsilon}}} \rangle = \sum_r c_r \underline{\underline{\boldsymbol{\varepsilon}}}_r \quad (31)$$

We have obviously : $\langle \underline{\underline{\mathbf{B}}} \rangle = \langle \underline{\underline{\mathbf{A}}} \rangle = \sum_r c_r \underline{\underline{\mathbf{B}}}_r = \sum_r c_r \underline{\underline{\mathbf{A}}}_r = \underline{\underline{\mathbf{I}}}$, where $\underline{\underline{\mathbf{I}}}$ denotes the fourth rank unit tensor.

3.1.2 Transformation Influence Functions

We now assume the presence of eigenstrain fields, that may represent consequences of various physical processes (thermal strains, plastic strains, transformation strains). However, at least if they conform with the small perturbation additive decomposition in (1), then, regardless of their origin, they may be considered as additional strains applied to the elastic aggregate, in superposition with the uniform overall strain. The local elastic constitutive equations (26) are replaced by :

$$\underline{\underline{\boldsymbol{\sigma}}}_r(x) = \underline{\underline{\mathbf{L}}}_r \left(\underline{\underline{\boldsymbol{\varepsilon}}}_r(x) - \underline{\underline{\boldsymbol{\mu}}}_r(x) \right) \quad \underline{\underline{\boldsymbol{\varepsilon}}}_r(x) = \underline{\underline{\mathbf{L}}}_r^{-1} \underline{\underline{\boldsymbol{\sigma}}}_r(x) + \underline{\underline{\boldsymbol{\mu}}}_r(x) \quad (32)$$

where $\underline{\underline{\boldsymbol{\mu}}}_r(x)$ represents a prescribed distribution of local eigenstrains. At the macroscale the overall elastic constitutive equations (27) now write :

$$\underline{\underline{\boldsymbol{\Sigma}}} = \underline{\underline{\bar{\mathbf{L}}}} \left(\underline{\underline{\mathbf{E}}} - \underline{\underline{\bar{\boldsymbol{\mu}}}} \right) \quad \underline{\underline{\mathbf{E}}} = \underline{\underline{\bar{\mathbf{L}}}}^{-1} \underline{\underline{\boldsymbol{\Sigma}}} + \underline{\underline{\bar{\boldsymbol{\mu}}}} \quad (33)$$

With the eigenstrain field represented by function $\underline{\underline{\boldsymbol{\mu}}}(x)$, the local strain field follows from the Lippman-Schwinger equation Bornert (2001) :

$$\underline{\underline{\boldsymbol{\varepsilon}}}(x) = \underline{\underline{\boldsymbol{\varepsilon}}}^o(x) - \int_V \underline{\underline{\Gamma}}(x, x') \left[\left(\underline{\underline{\mathbf{L}}}(x') - \underline{\underline{\bar{\mathbf{L}}}}^o \right) \underline{\underline{\boldsymbol{\varepsilon}}}(x') - \underline{\underline{\mathbf{L}}}(x') \underline{\underline{\boldsymbol{\mu}}}(x') \right] dx' \quad (34)$$

in which $\underline{\underline{\varepsilon}}^o(x)$ denotes the strain field (uniform) that would exist in a comparison homogeneous medium of elastic stiffness $\underline{\underline{\mathbb{L}}}^o$ under the same boundary conditions. The kernel $\underline{\underline{\mathbb{T}}}$ is defined by :

$$\Gamma_{ijkl}(x, x') = -\frac{1}{2} [G_{ik,jl}(x, x') + G_{jl,il}(x, x')] \quad (35)$$

where G_{ik} is the Green function of the homogeneous medium $\underline{\underline{\mathbb{L}}}^o$ that satisfy :

$$L_{ijkl}^o G_{kp,lj}(x, x') + \delta_{ip} \delta(x - x') = 0 \quad \forall x, x' \in V \quad (36)$$

where δ_{ip} is the Kronecker symbol, and $\delta(x - x')$ is the Dirac function. Exemples of such forms can be found in papers by Levin (1976), Willis (1978), Willis (1981). In some cases (Molinari et al. (1997)) there is an additional term $\underline{\underline{\mathbb{L}}}^o \underline{\underline{\mu}}$ to the local eigenstress $\underline{\underline{\mathbb{L}}}(x') \underline{\underline{\mu}}(x')$, but that does not change the results that will be used below.

The only assumption made by Dvorak and Benveniste (1992) is that eigenstrain fields are represented by distributions that are piecewise uniform, either in the phases or in the local subvolumes V_r within those phases. The total strain (stress) caused in V_s by the uniform overall strain $\underline{\underline{\mathbb{E}}}$ (stress $\underline{\underline{\Sigma}}$) and piecewise uniform eigenstrains $\underline{\underline{\mu}}_r$ is assumed in the following form :

$$\underline{\underline{\varepsilon}}_s(x) = \underline{\underline{\mathbb{A}}}_s(x) \underline{\underline{\mathbb{E}}} + \sum_r \underline{\underline{\mathbb{D}}}_{sr}(x) \underline{\underline{\mu}}_r \quad (37)$$

$$\underline{\underline{\sigma}}_s(x) = \underline{\underline{\mathbb{B}}}_s(x) \underline{\underline{\Sigma}} - \sum_r \underline{\underline{\mathbb{F}}}_{sr}(x) \underline{\underline{\mathbb{L}}}_r \underline{\underline{\mu}}_r \quad (38)$$

The $\underline{\underline{\mathbb{D}}}_{ss}(x)$ and $\underline{\underline{\mathbb{D}}}_{sr}(x)$ are, respectively, the self-induced and transmitted eigenstrain influence functions. The $\underline{\underline{\mathbb{F}}}_{ss}(x)$ and $\underline{\underline{\mathbb{F}}}_{sr}(x)$ are the corresponding eigenstress influence functions. Collectively they are called the *transformation influence functions*. Let us note that, in the standard use of this method, the eigenstrains $\underline{\underline{\mu}}_r$ are the sum of the plastic strain and thermal expansion in each sub-volume V_r .

Let us give now the relation between the local and overall eigenstrains. This can be done by invoking the elastic reciprocal theorem. The complete demonstration is given by Dvorak and Benveniste (1992) and recovers the relations due to Mandel (1964) and Levin (1967) :

$$\underline{\underline{\mu}} = \langle \underline{\underline{\mathbb{B}}}^T \underline{\underline{\mu}} \rangle = \frac{1}{V} \sum_r \int_{V_r} \underline{\underline{\mathbb{B}}}_r^T(x) \underline{\underline{\mu}}_r(x) dx \quad (39)$$

which reduces to : $\underline{\underline{\mu}} = \sum_r c_r \underline{\underline{\mathbb{B}}}_r^T \underline{\underline{\mu}}_r$ for piecewise uniform eigenstrain $\underline{\underline{\mu}}_r$ (uniform on the sub-volume V_r).

3.1.3 Some Properties and Applications

Firstable let us give the general relationship between $\underline{\underline{\mathbb{D}}}_{sr}$ and $\underline{\underline{\mathbb{F}}}_{sr}$. It comes out by expressing $\underline{\underline{\sigma}}_s(x)$ from (26), incorporating (37) and (33), taking account of (39), and identifying with (38) :

$$\underline{\underline{\mathbb{F}}}_{sr}(x) = \underline{\underline{\mathbb{L}}}_s \left[\delta_{sr} \underline{\underline{\mathbb{I}}} - c_r \underline{\underline{\mathbb{A}}}_s(x) \underline{\underline{\mathbb{B}}}_r^T(x) - \underline{\underline{\mathbb{D}}}_{sr}(x) \right] \underline{\underline{\mathbb{L}}}_r^{-1} \quad (40)$$

Examining different particular cases that involve piecewise uniform fields Dvorak and Benveniste (1992), one obtain the following properties for the transformation influence functions :

$$\sum_r \underline{\underline{\mathbb{D}}}_{sr}(x) = \underline{\underline{\mathbb{I}}} - \underline{\underline{\mathbb{A}}}_s(x) \quad \sum_r \underline{\underline{\mathbb{F}}}_{sr}(x) = \underline{\underline{\mathbb{I}}} - \underline{\underline{\mathbb{B}}}_s(x) \quad (41)$$

$$\sum_r \underline{\underline{\mathbb{D}}}_{sr}(x) \underline{\underline{\mathbb{L}}}_r^{-1} = 0 \quad \sum_r \underline{\underline{\mathbb{F}}}_{sr}(x) \underline{\underline{\mathbb{L}}}_r = 0 \quad (42)$$

$$c_s \underline{\underline{\mathbb{L}}}_s \underline{\underline{\mathbb{D}}}_{sr} = c_r \underline{\underline{\mathbb{D}}}_{rs}^T \underline{\underline{\mathbb{L}}}_r \quad c_s \underline{\underline{\mathbb{F}}}_{sr} \underline{\underline{\mathbb{L}}}_r = c_r \underline{\underline{\mathbb{L}}}_s \underline{\underline{\mathbb{F}}}_{rs}^T \quad (43)$$

$$\sum_r c_r \underline{\underline{\mathbf{D}}}_{rs} = 0 \quad \sum_r c_r \underline{\underline{\mathbf{F}}}_{rs} = 0 \quad (44)$$

Relation (43) was obtained by invoking the elastic reciprocal theorem. The last equalities (44) easily follow from the definition of overall stress and strain in (31), used in (37) and (38), where each local eigenstrain $\underline{\underline{\mu}}_r$ can be chosen independently. Let us note that in (43) and (44), $\underline{\underline{\mathbf{D}}}_{sr}$ and $\underline{\underline{\mathbf{D}}}_{rs}$ denote respectively the averages of $\underline{\underline{\mathbf{D}}}_{sr}(x)$ and $\underline{\underline{\mathbf{D}}}_{rs}(x)$ respectively on V_s and V_r .

The above localization relations can be exploited either for composite materials or for more random microstructures. In the first case, thanks to the quasi-periodic structure, we can use numerical methods Dvorak et al. (1994), Pottier (1998), Chaboche et al. (1999), based on periodic homogenization techniques, to determine all the concentration and transformation influence tensors. When a sufficient number of sub-volumes is used in the local geometrical and material description, one recovers the properties of the continuous local field solutions and a correct modeling both at the overall scale and at the microscale. In the second one, the method can be used in a two phase model, considering only average quantities over each phase and Eshelby based closed form solutions for the various concentration and influence tensors (a multiphase modeling is also available, provided all inclusions have the same shape and same orientation Dvorak (1992)). In this case the solution appears much too stiff in the plastic regime, as discussed in many different papers Zaoui and Raphanel (1993), Suquet (1996), Zaoui and Masson (1998), and it has been the subject of researching improved methods based on secant or tangent or affine or second order approximations of the elasto(visco)plastic local and overall behaviors Molinari et al. (1997), Masson and Zaoui (1999), Ponte Castañeda and Suquet (1995), Masson et al. (2000). One possibility of correction of the same approach for a limited number of sub-volumes was considered by Pottier Pottier (1998), Chaboche et al. (2001).

Let us remark the recent generalization made by Michel et al. (2000), introducing non uniform shape functions in place of piecewise uniform fields. This method, called NTFA (*Nonuniform Transformation Field Analysis*), offers additional possibilities, with a low number of independent functions, and can also lead to energy considerations similar to those developed in section 3.2.

3.1.4 A More General Continuous Description

In fact, the form of localization equations (37), (38), with piecewise uniform eigenstrains, was already formulated within a continuous description. We re-discovered it into papers by Suquet (1982), Nguyen (1988), but it was probably much earlier. The main arguments are twofold : (i) - formulate the localization problem in the RVE as an elasticity structural boundary-value problem (assuming zero body forces), as we usually do in periodic homogenization techniques, and (ii) - invoke Hill's Lemma that is satisfied for any local stress and strain fields $\underline{\underline{\sigma}}$, $\underline{\underline{\varepsilon}}$ such that :

- $\underline{\underline{\varepsilon}}$ is kinematically admissible, K.A.
i.e. : $\underline{\underline{\varepsilon}} = (\nabla \underline{\mathbf{u}})$ in V
- $\underline{\underline{\sigma}}$ is statically admissible, S.A.
i.e. : $\text{div} \underline{\underline{\sigma}} = 0$ in V
- $\underline{\underline{\sigma}}$, $\underline{\underline{\varepsilon}}$ satisfy on ∂V the localization condition
(Hill's macro-homogeneity condition)

Hill's Lemma is then expressed by the condition :

$$\langle \underline{\underline{\sigma}} \mid \underline{\underline{\varepsilon}} \rangle = \langle \underline{\underline{\sigma}} \mid \underline{\underline{\varepsilon}} \rangle \quad (45)$$

We take from Nguyen (1988) the following developments, using present Dvorak's notations, but a more general writing. We limit ourselves to isothermal plasticity (the only eigenstrain is the plastic strain $\underline{\underline{\varepsilon}}^p$). In the periodic case, the strain localization problem can be explicitly written as :

$\underline{\mathbf{E}}, \underline{\boldsymbol{\varepsilon}}^p$ are given ;
Find $\underline{\boldsymbol{\sigma}}, \underline{\boldsymbol{\varepsilon}}$ such that :

- $\underline{\boldsymbol{\varepsilon}} = (\nabla \underline{\mathbf{u}})$
- $\text{div} \underline{\boldsymbol{\sigma}} = 0$ in V
- $\underline{\boldsymbol{\sigma}} = \underline{\mathbf{L}}(\underline{\boldsymbol{\varepsilon}} - \underline{\boldsymbol{\varepsilon}}^p)$
- $\underline{\boldsymbol{\sigma}}, \underline{\boldsymbol{\varepsilon}}$ periodic on ∂V
- $\langle \underline{\boldsymbol{\sigma}} \rangle = \underline{\boldsymbol{\Sigma}}, \langle \underline{\boldsymbol{\varepsilon}} \rangle = \underline{\mathbf{E}}$

This is a linear problem with residual strains and appropriate boundary conditions. It is then interesting to introduce the following decomposition of stress and strain. We begin by the strain decomposition, in which the discrete strain localization condition (37) is replaced by its continuous expression :

$$\underline{\boldsymbol{\varepsilon}} = \underline{\mathbf{A}} \underline{\mathbf{E}} + \underline{\mathbf{D}} \underline{\boldsymbol{\varepsilon}}^p \quad (47)$$

Here $\underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\varepsilon}}^p, \underline{\mathbf{A}}, \underline{\mathbf{D}}$ stand for field expressions. Moreover $\underline{\mathbf{D}}$ is an integral operator, so that (47) reads more explicitly :

$$\underline{\boldsymbol{\varepsilon}}(x) = \underline{\mathbf{A}}(x) \underline{\mathbf{E}} + \int_V \underline{\mathbf{D}}(x, x') \underline{\boldsymbol{\varepsilon}}^p(x') dx' \quad (48)$$

an expression that resembles (34). In eqn. (47), as well as in the developments below, we suppressed the conventional notation $\underline{\mathbf{D}} * \underline{\boldsymbol{\varepsilon}}^p$ for the convolution. Similarly we write for the stress localization :

$$\underline{\boldsymbol{\sigma}} = \underline{\mathbf{B}} \underline{\boldsymbol{\Sigma}} - \underline{\mathbf{F}} \underline{\mathbf{L}} \underline{\boldsymbol{\varepsilon}}^p \quad (49)$$

with similar meanings for the operators. Such decompositions have the following interesting properties. For the strain : $\underline{\boldsymbol{\varepsilon}} = \underline{\mathbf{A}} \underline{\mathbf{E}}$ is kinematically admissible (KA) provided it corresponds to the elastic solution of the boundary value problem ; $\underline{\mathbf{L}} \underline{\boldsymbol{\varepsilon}} = \underline{\mathbf{L}} \underline{\mathbf{A}} \underline{\mathbf{E}}$ is statically admissible (SA). As the difference between the true local strain solution and the elastic one $\underline{\boldsymbol{\varepsilon}} = \underline{\mathbf{D}} \underline{\boldsymbol{\varepsilon}}^p$ is also KA and $\underline{\mathbf{L}}(\underline{\boldsymbol{\varepsilon}} - \underline{\boldsymbol{\varepsilon}}^p) = \underline{\mathbf{L}}(\underline{\mathbf{D}} - \underline{\mathbf{I}}) \underline{\boldsymbol{\varepsilon}}^p$ is also SA. Here $\underline{\mathbf{D}}$ denotes the linear operator of strain incompatibility. Similarly, we learn that $\underline{\boldsymbol{\Sigma}} = \underline{\mathbf{B}} \underline{\boldsymbol{\Sigma}}$ is SA, as the elastic solution, and $\underline{\mathbf{L}}^{-1} \underline{\boldsymbol{\Sigma}} = \underline{\mathbf{L}}^{-1} \underline{\mathbf{B}} \underline{\boldsymbol{\Sigma}}$ is KA. Moreover $\underline{\mathbf{r}} = -\underline{\mathbf{F}} \underline{\mathbf{L}} \underline{\boldsymbol{\varepsilon}}^p$ is SA as the difference of two SA fields. Here $\underline{\mathbf{R}} = \underline{\mathbf{F}} \underline{\mathbf{L}}$ is the linear operator of stress incompatibility.

Note that $\underline{\mathbf{D}}$ and $\underline{\mathbf{R}} = \underline{\mathbf{F}} \underline{\mathbf{L}}$ are also well known in the mathematical theory of dislocations. Operator $\underline{\mathbf{D}}$ generates the strain response from a given incompatibility. Very often $\underline{\mathbf{r}} = \underline{\mathbf{R}} \underline{\boldsymbol{\varepsilon}}^p$ is also called the residual stress field. Obviously we have the following properties :

$$\langle \underline{\boldsymbol{\varepsilon}} \rangle = \langle \underline{\mathbf{D}} \underline{\boldsymbol{\varepsilon}}^p \rangle = 0 \quad \langle \underline{\mathbf{r}} \rangle = \langle \underline{\mathbf{F}} \underline{\mathbf{L}} \underline{\boldsymbol{\varepsilon}}^p \rangle = 0 \quad (50)$$

that are also contained into eqs (44). There is now a simple way to obtain eqs (39), by using Hill's Lemma. We start from (47) and apply the constitutive equation (46) :

$$\underline{\boldsymbol{\sigma}} = \underline{\mathbf{L}} \underline{\mathbf{A}} \underline{\mathbf{E}} + \underline{\mathbf{L}} (\underline{\mathbf{D}} - \underline{\mathbf{I}}) \underline{\boldsymbol{\varepsilon}}^p \quad (51)$$

which average must be :

$$\underline{\boldsymbol{\Sigma}} = \langle \underline{\boldsymbol{\sigma}} \rangle = \langle \underline{\mathbf{L}} \underline{\mathbf{A}} \rangle \underline{\mathbf{E}} + \langle \underline{\mathbf{L}} (\underline{\mathbf{D}} - \underline{\mathbf{I}}) \underline{\boldsymbol{\varepsilon}}^p \rangle \quad (52)$$

We recover $\underline{\mathbf{L}} = \langle \underline{\mathbf{L}} \underline{\mathbf{A}} \rangle$ for the purely elastic behaviour and, provided the overall elastic constitutive equation

$$\underline{\boldsymbol{\Sigma}} = \underline{\mathbf{L}} (\underline{\mathbf{E}} - \underline{\boldsymbol{\varepsilon}}^p) \quad (53)$$

we obtain :

$$\underline{\mathbf{L}} \underline{\boldsymbol{\varepsilon}}^p = - \langle \underline{\mathbf{L}} (\underline{\mathbf{D}} - \underline{\mathbf{I}}) \underline{\boldsymbol{\varepsilon}}^p \rangle \quad (54)$$

From Hill's Lemma $\langle \rho \rangle = \langle \underline{\underline{\mathbf{A}}}^T \rho \rangle$ if ρ is SA (provided $\underline{\underline{\mathbf{A}}}$ is KA). Thus, because $\underline{\underline{\mathbf{L}}} (\underline{\underline{\mathbf{D}}} - \underline{\underline{\mathbf{I}}})$ is SA, the second member can also be written $\langle \underline{\underline{\mathbf{A}}}^T \underline{\underline{\mathbf{L}}} (\underline{\underline{\mathbf{D}}} - \underline{\underline{\mathbf{I}}}) \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle$. Using now the equality (29), and multiplying by $\underline{\underline{\mathbf{L}}}^{-1}$, we obtain :

$$\underline{\underline{\mathbf{E}}}^p = \langle \underline{\underline{\mathbf{B}}}^T \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle - \langle \underline{\underline{\mathbf{B}}}^T \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle \quad (55)$$

However $\underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p$ is KA and $\underline{\underline{\mathbf{B}}}$ is SA, so that the last term also writes $\langle \underline{\underline{\mathbf{B}}}^T \rangle \langle \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle$. Provided $\langle \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle = 0$, we finally obtain the Levin-Mandel result :

$$\underline{\underline{\mathbf{E}}}^p = \langle \underline{\underline{\mathbf{B}}}^T \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle \quad (56)$$

Let us note the following equalities, also given from Hill's Lemma, that prove the symmetry of overall stiffness and compliance :

$$\underline{\underline{\mathbf{L}}} = \langle \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{A}}} \rangle = \langle \underline{\underline{\mathbf{A}}}^T \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{A}}} \rangle \quad \underline{\underline{\mathbf{L}}}^{-1} = \langle \underline{\underline{\mathbf{L}}}^{-1} \underline{\underline{\mathbf{B}}} \rangle = \langle \underline{\underline{\mathbf{B}}}^T \underline{\underline{\mathbf{L}}}^{-1} \underline{\underline{\mathbf{B}}} \rangle \quad (57)$$

3.2 Energy Considerations

3.2.1 Local to Overall State Potential

Let us assume a local free energy in the form :

$$\psi(\underline{\underline{\boldsymbol{\varepsilon}}}, \underline{\underline{\boldsymbol{\varepsilon}}}^p, a_j) = \frac{1}{2} (\underline{\underline{\boldsymbol{\varepsilon}}} - \underline{\underline{\boldsymbol{\varepsilon}}}^p) \underline{\underline{\mathbf{L}}} (\underline{\underline{\boldsymbol{\varepsilon}}} - \underline{\underline{\boldsymbol{\varepsilon}}}^p) + \psi_p(a_j) \quad (58)$$

By integrating, we will show the corresponding form for the overall free energy :

$$\bar{\psi} = \langle \psi \rangle = \frac{1}{2} \langle (\underline{\underline{\mathbf{A}}} \underline{\underline{\mathbf{E}}} + \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p)^T \underline{\underline{\mathbf{L}}} (\underline{\underline{\mathbf{A}}} \underline{\underline{\mathbf{E}}} + \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p) \rangle + \bar{\psi}_p(a) \quad (59)$$

where $\underline{\underline{\mathbf{D}}}$ stands for $\underline{\underline{\mathbf{D}}} - \underline{\underline{\mathbf{I}}}$. Note, with the Dvorak discrete notations, that $\underline{\underline{\mathbf{D}}}_{rs} = \underline{\underline{\mathbf{D}}}_{rs} - \underline{\underline{\mathbf{I}}}_{rs}$. After developing we obtain three terms :

$$\bar{\psi} = \frac{1}{2} \underline{\underline{\mathbf{E}}} \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}} + \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{A}}} \rangle \underline{\underline{\mathbf{E}}} + \frac{1}{2} \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle + \bar{\psi}_p(a) \quad (60)$$

The second term is modified by taking into account (56) :

$$\bar{\psi}_2 = \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{B}}} \rangle \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}} = \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{B}}} \rangle \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}} - \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{B}}} \rangle \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}} \quad (61)$$

Now we observe that $\underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p$ is KA and $\underline{\underline{\mathbf{B}}}$ is SA, so that we can write the first term in (61) as $\langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \rangle \langle \underline{\underline{\mathbf{B}}} \rangle \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}}$, that vanishes from (50). Using (50) and (56) in (60), we finally found :

$$\bar{\psi} = \frac{1}{2} \underline{\underline{\mathbf{E}}} \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{E}}} - \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{L}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p + \frac{1}{2} \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{L}}} \underline{\underline{\mathbf{D}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle + \bar{\psi}_p(a) \quad (62)$$

which can also be rewritten :

$$\bar{\psi} = \frac{1}{2} (\underline{\underline{\mathbf{E}}} - \underline{\underline{\boldsymbol{\varepsilon}}}^p) \underline{\underline{\mathbf{L}}} (\underline{\underline{\mathbf{E}}} - \underline{\underline{\boldsymbol{\varepsilon}}}^p) - \frac{1}{2} \underline{\underline{\boldsymbol{\varepsilon}}}^p \underline{\underline{\mathbf{L}}} \underline{\underline{\boldsymbol{\varepsilon}}}^p + \frac{1}{2} \langle \underline{\underline{\boldsymbol{\varepsilon}}}^p (\underline{\underline{\mathbf{D}}}^T - \underline{\underline{\mathbf{I}}}) \underline{\underline{\mathbf{L}}} (\underline{\underline{\mathbf{D}}} - \underline{\underline{\mathbf{I}}}) \underline{\underline{\boldsymbol{\varepsilon}}}^p \rangle + \bar{\psi}_p(a) \quad (63)$$

The overall free energy can be obtained by another way, averaging the complementary form of the local energy :

$$\psi(\underline{\underline{\boldsymbol{\sigma}}}, a_j) = \frac{1}{2} \underline{\underline{\boldsymbol{\sigma}}} \underline{\underline{\mathbf{L}}}^{-1} \underline{\underline{\boldsymbol{\sigma}}} + \psi_p(a_j) \quad (64)$$

After replacing $\underline{\sigma}$ by (49), and taking into account $\langle \underline{\mathbf{B}}^T \underline{\mathbf{A}} \rangle = \underline{\mathbf{I}}$ and (57), we obtain :

$$\bar{\psi} = \langle \psi \rangle = \frac{1}{2} \underline{\Sigma} \underline{\bar{\mathbf{L}}}^{-1} \underline{\Sigma} - \left\langle \underline{\varepsilon}^p \underline{\mathbf{L}} \underline{\bar{\mathbf{F}}}^T \underline{\mathbf{L}}^{-1} \underline{\mathbf{B}} \right\rangle \underline{\Sigma} + \frac{1}{2} \left\langle \underline{\varepsilon}^p \underline{\mathbf{L}} \underline{\bar{\mathbf{F}}}^T \underline{\mathbf{L}}^{-1} \underline{\mathbf{F}} \underline{\mathbf{L}} \underline{\varepsilon}^p \right\rangle + \bar{\psi}_p(a) \quad (65)$$

In this expression the intermediate term vanishes from Hill's Lemma. In effect, it expresses successively, using (29) : $\langle \underline{\varepsilon}^p \underline{\mathbf{L}} \underline{\bar{\mathbf{F}}}^T \underline{\mathbf{L}}^{-1} \underline{\mathbf{B}} \rangle = \langle \underline{\varepsilon}^p \underline{\mathbf{L}} \underline{\bar{\mathbf{F}}}^T \underline{\mathbf{A}} \rangle \underline{\bar{\mathbf{L}}}^{-1} = \langle \underline{\varepsilon}^p \underline{\mathbf{L}} \underline{\bar{\mathbf{F}}}^T \rangle \langle \underline{\mathbf{A}} \rangle \underline{\bar{\mathbf{L}}}^{-1} = 0$, because $\underline{\mathbf{A}}$ is KA, $\underline{\mathbf{r}} = -\underline{\mathbf{F}} \underline{\mathbf{L}} \underline{\varepsilon}^p$ is SA and its average vanishes. Finally, transforming the last term and using (53), we find :

$$\bar{\psi} = \frac{1}{2} (\underline{\mathbf{E}} - \underline{\mathbf{E}}^p) \underline{\bar{\mathbf{L}}} (\underline{\mathbf{E}} - \underline{\mathbf{E}}^p) + \frac{1}{2} \left\langle \underline{\mathbf{r}} \underline{\mathbf{L}}^{-1} \underline{\mathbf{r}} \right\rangle + \bar{\psi}_p(a) \quad (66)$$

Comparison with (63) clearly shows that the second and third terms in (63) correspond exactly with the residual stresses associated with the non uniformity of local plastic strains. Let us note that the equality can also be obtained directly, using relation (40). It means that only the quadratic form (63) for the overall potential is able to correctly separate the independent variables. The equivalent expression (62) does not separate correctly the independent effects.

3.2.2 Dissipations

The overall dissipation can be written in a differential form as :

$$\delta\Phi = \underline{\Sigma} \delta\underline{\mathbf{E}} - \delta\bar{\psi}_p = \underline{\Sigma} \delta\underline{\mathbf{E}}^p + \underline{\mathbf{E}}^p \underline{\bar{\mathbf{L}}} \delta\underline{\mathbf{E}}^p - \left\langle \underline{\varepsilon}^p (\underline{\mathbf{D}}^T - \underline{\mathbf{I}}) \underline{\mathbf{L}} (\underline{\mathbf{D}} - \underline{\mathbf{I}}) \delta\underline{\varepsilon}^p \right\rangle - \delta\bar{\psi}_p \quad (67)$$

using form (63) for $\bar{\psi}$. We have to take into account the constraint (56) and, thanks to Hill's Lemma, the last term simplifies. We then have :

$$\delta\Phi = \underline{\Sigma} \delta\underline{\mathbf{E}}^p + \underline{\mathbf{E}}^p \underline{\bar{\mathbf{L}}} \left\langle \underline{\mathbf{B}}^T \delta\underline{\varepsilon}^p \right\rangle + \left\langle \underline{\varepsilon}^p (\underline{\mathbf{D}}^T - \underline{\mathbf{I}}) \underline{\mathbf{L}} \delta\underline{\varepsilon}^p \right\rangle - \delta\bar{\psi}_p \quad (68)$$

Now, let us recall the residual stress field :

$$\begin{aligned} \underline{\mathbf{r}} &= \underline{\sigma} - \underline{\mathbf{B}} \underline{\Sigma} = \underline{\mathbf{L}} (\underline{\varepsilon} - \underline{\varepsilon}^p) - \underline{\mathbf{B}} \underline{\Sigma} \\ &= \underline{\mathbf{L}} \left(\underline{\mathbf{A}} \underline{\mathbf{E}} + \underline{\mathbf{D}} \underline{\varepsilon}^p - \underline{\varepsilon}^p \right) - \underline{\mathbf{B}} \underline{\bar{\mathbf{L}}} (\underline{\mathbf{E}} - \underline{\mathbf{E}}^p) = \underline{\mathbf{L}} (\underline{\mathbf{D}} - \underline{\mathbf{I}}) \underline{\varepsilon}^p + \underline{\mathbf{B}} \underline{\bar{\mathbf{L}}} \underline{\mathbf{E}}^p \end{aligned} \quad (69)$$

that shows the dissipation becomes :

$$\delta\Phi = \underline{\Sigma} \delta\underline{\mathbf{E}}^p + \left\langle \underline{\mathbf{r}} \delta\underline{\varepsilon}^p \right\rangle - \delta\bar{\psi}_p \quad (70)$$

including three terms : the first one is the plastic power (or inelastic external power), the second one the power dissipated by residual stresses (or second order internal stresses), though the third term, not explicitly defined, corresponds to the power dissipated at the lower scales, by the third order internal stresses.

The above expression (70) for dissipation, with the residual stress internal power, confirms that the second term in (63), expressed in $\underline{\mathbf{E}}^p$, must in fact be considered as depending on the microscale variables $\underline{\varepsilon}^p$.

3.2.3 Consequencies for the State Potential

We have shown two equivalent forms, (63) and (66), for the overall state potential expressed in terms of overall total and plastic strains. In fact, the presence in (66) of the stored energy associated with residual stresses and non uniform local strains demonstrates that the second term in (63) has to be interpreted in terms of local quantities. It shows that, in a macroscopic constitutive equation, the state potential has to be taken as quadratic in the elastic strain $\underline{\mathbf{E}} - \underline{\mathbf{E}}^p$. The additional stored energy (here representing the role of residual stresses) corresponds then to additional state variables (independent variables at the macroscale). We can interpret the residual stress term in (66) as corresponding to kinematic hardening (second order residual stresses, at the level of the grains in a

polycrystal). The third term in (66), $\bar{\psi}_p(a)$, then corresponds to isotropic hardening : it is more or less related to internal variables of the microscale level, that is, in a polycrystal, to the intragranular stresses and to the dislocation substructures.

The above discussion is generally accepted. Most of the micromechanics based theories use an overall potential of the form (66), with a quadratic term expressed in the overall elastic strain. Surprisingly it is not so general for the thermoelastic theory, where potential forms are often like :

$$\bar{\psi} = \frac{1}{2} \mathbf{E} \bar{\mathbb{L}} \mathbf{E} - \frac{1}{2} \mathbf{E}^\theta \bar{\mathbb{L}} \mathbf{E} + \bar{\psi}_\theta(T) \quad (71)$$

where $\mathbf{E}^\theta = \alpha \theta = \alpha (T - T_o)$ is the thermal expansion and $\bar{\psi}_\theta(T)$ is the part of the free energy not related to the strain. This last term is often taken in the form $\bar{\psi}_\theta = C^\varepsilon \left(T_o \ln \frac{T}{T_o} - \theta \right)$ Freed and Chaboche (1989) or of its first order approximation $\bar{\psi}_\theta = -\frac{C^\varepsilon}{2T_o} \theta^2$ Lemaître and Chaboche (1985).

In fact, the micromechanics based method shows us that the form (71) should be replaced by a form quadratic in the mechanical part of the thermoelastic strain $\mathbf{E}^e = \mathbf{E} - \mathbf{E}^\theta$, with $\mathbf{E}^\theta = \langle \mathbf{B}^T \boldsymbol{\varepsilon}^\theta \rangle$:

$$\begin{aligned} \bar{\psi} = & \frac{1}{2} (\mathbf{E} - \mathbf{E}^\theta) \bar{\mathbb{L}} (\mathbf{E} - \mathbf{E}^\theta) - \frac{1}{2} \mathbf{E}^\theta \bar{\mathbb{L}} \mathbf{E}^\theta \\ & + \frac{1}{2} \langle \boldsymbol{\varepsilon}^\theta (\mathbf{D}^T - \mathbf{I}) \bar{\mathbb{L}} (\mathbf{D} - \mathbf{I}) \boldsymbol{\varepsilon}^\theta \rangle + \bar{\psi}_\theta(T) \end{aligned} \quad (72)$$

More conveniently, with residual stresses associated to non uniform elastic constants or thermal expansion coefficients, we should have :

$$\bar{\psi} = \frac{1}{2} (\mathbf{E} - \mathbf{E}^\theta) \bar{\mathbb{L}} (\mathbf{E} - \mathbf{E}^\theta) + \frac{1}{2} \langle \boldsymbol{\varepsilon}^\theta \bar{\mathbb{L}}^{-1} \boldsymbol{\varepsilon}^\theta \rangle + \bar{\psi}_\theta(T) \quad (73)$$

Then, macroscopically speaking, for the overall theory, thermodynamic potential (Helmholtz free energy) should be quadratic in the mechanical elastic strain, and contain an additional term quadratic in the temperature (at least if we assume the temperature as locally uniform inside the RVE) :

$$\bar{\psi} = \frac{1}{2} (\mathbf{E} - \mathbf{E}^\theta) \bar{\mathbb{L}} (\mathbf{E} - \mathbf{E}^\theta) + \bar{\psi}_\theta^*(\theta) + \bar{\psi}_\theta(T) \quad (74)$$

Let us note that such a form was used in Chaboche (1978), with a completely independent argument, related to the simplicity, in order to take into account the damage effects in the elastic behaviour.

4 Conclusion

Continuum Thermodynamics of Irreversible Processes has been revisited, based on the local state hypothesis and the use of internal state variables. Both the macroscopic constitutive framework and micromechanics based relations have been discussed :

1. From the macroscopic point of view, the classical framework of GSM, Generalized Standard Models, was discussed, showing some of the too strict restrictions that concern both the introduction of non linear kinematic hardening and the development of Continuum Damage Mechanics equations.
2. A slightly less restrictive approach is proposed, within a Quasi-Standard Model, that considers several independent dissipative potentials and several independent multiplying functions, associated with the various processes, plasticity and hardening, static recovery and aging, damage effects.
3. Concerning micromechanics and scale change methods, we have recalled the Transformation Field Analysis proposed by Dvorak and co-workers Dvorak and Benveniste (1992), Dvorak (1992). It appears as a good tool, even if it needs improvements and corrections in cases where only a few sub-volumes are considered Chaboche et al. (1999). In fact the same localization relations were previously given formally, for instance in the work by Suquet (1982) or Nguyen (1988).

4. From these micromechanics relationships one obtain the expression for the overall free energy. The fact that it expresses as a quadratic function of elastic strain, to which is added the stored energy associated with internal residual stresses, is particularly underlined. The thermoelastic free energy is also discussed, in which a quadratic function of the mechanical elastic strain appears similarly. Such a quadratic expression is not always well considered and this is a point that merits further attention.
5. Other related aspects were not considered in the present paper, and are briefly summarized here :
 - The thermodynamic framework presents the advantage to separate the plastic work into the part that is dissipated as heat and the one that is stored in the material (by the internal stresses). Previous works Chaboche (1993), Chaboche (1996) have shown its ability to correctly represent mechanical and thermal measurements Chrysochoos (1987), which means the correct modelling of dissipated energy.
 - The use of the rate of observable variables (total strain rate or elastic strain rate or stress rate) in the evolution equations for internal variables introduces some shortcomings Malmberg (1990), Chaboche (1996), that are still subject to discussion Krempl (1996).
 - The temperature rate does appear in the back stress rate equation, but only as a consequence of the temperature dependency of hardening moduli. This dependency is directly obtained from the thermodynamic framework and its violation can induce abnormal and unacceptable mechanical responses, that have been discussed in Chaboche (1993), Ohno and Wang (1992).
 - Concerning damage effect modelling, the important aspects related to damage deactivation effects are the subject of some difficulties : depending on the deactivation rule chosen, there are needs to define differently the plastic strain, modifying the "unloaded configuration", as was discussed in Chaboche et al. (1998).

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