IL NUOVO CIMENTO Vol. 32 C, N. 1 Gennaio-Febbraio 2009
DOI 10.1393/ncc/i2009-10340-9

Colloquia: GCM8

Thermodynamics of quasi–rate-independent inelastic micromorphic polycrystals

M. Mićunović(*)

Masinski fakultet, Univerzitet Kragujevac - Sestre Janjica 6a, 34000 Kragujevac, Serbia

(ricevuto il 3 Aprile 2009; pubblicato online il 15 Giugno 2009)

Summary. — The paper deals with some new evolution equations for gradient viscoplasticity. Geometric and kinematic aspects of intragranular as well as intergranular plastic deformation of polycrystals are briefly discussed. Low-order inelastic polycrystals with homogeneous grain strains are considered. A homogenization of total, plastic and elastic strains has been done. By tensor representation applied to 3-tensors as well as to 2-tensors a simple case of gradient theory is formulated with a new evolution equation for plastic stretching gradient. An endochronic thermodynamics covering creep-plasticity interaction is applied.

PACS 46.35.+z – Viscoelasticity, plasticity, viscoplasticity.
PACS 61.72.Bb – Theories and models of crystal defects.
PACS 81.70.Bt – Mechanical testing, impact tests, static and dynamic loads.

1. – Introduction

The objective of this work is to pursue further research towards a simple yet realistic description of polycrystal behavior of metals extending considerations presented in the paper [1]. The contents of [1] are here briefly reviewed if necessary and the accent is put into an extension of evolution equations derived in [1] to cover also gradient of plastic stretching. In general, the residual stresses exist even when external forces are absent, and due to discontinuous change of orientation of neighbouring grain lattices it is natural to expect also couple stresses. Of special interest would be to connect material constants for stress and couple stress achieving their minimal number to be calibrated from specially designed experiments. Another issue of great importance is the question how to insert a grain larger than its available "hole" in the material of the considered body. The usual answer to this question is obtained by the so-called self-consistent methods (cf. [2]). Due to brevity of exposition it is not considered here. Details are given in [3]. The third issue

(*) E-mail: mmicun@kg.ac.yu

is proper geometry of the considered thermo-inelastic strain history for a polycrystalline body. It is almost completely squeezed here since it was analyzed in detail in [1].

In this paper we use direct notation with $\mathcal{A}\circ\mathcal{B}\equiv(\mathcal{A})_{abc}(\mathcal{B})^{abc}$, $\mathbf{A}:\mathbf{B}\equiv(\mathbf{A})_{ab}(\mathbf{B})^{ab}$ and $(\mathbf{AB})^{a}_{\cdot b}\equiv(\mathbf{A})^{ac}(\mathbf{B})_{cb}$. The other symbols are standard.

2. – Preliminaries

As a prerequisite, a correct geometric description of an inelastic deformation process analyzed is necessary. Consider a polycrystalline body in a real configuration $(k(t))$ with dislocations and an inhomogeneous temperature field $T(X,t)$ (where t stands for time and X for the considered particle of the body) subject to surface tractions. Corresponding to $(k(t))$ there exists, usually, an initial reference configuration $(k(t_0))$ with (differently distributed) dislocations at a homogeneous temperature T_0 without surface tractions. Due to these defects such a configuration is not stress-free but contains an equilibrated residual stress (often named as "back-stress"). It is generally accepted that linear mapping function $\mathbf{F}(.,t):(k(t_0))\rightarrow(k(t))$ is compatible second-rank *total deformation gradient tensor*. Here time t as a scalar parameter allows for a family of deformed configurations (k). In the papers dealing with continuum representations of dislocation distributions configuration $(k(t))$ is imagined to be cut into small elements denoted by $(n(t))$, these being subsequently brought to the temperature of $(k(t_0))$ free of neighbors. The deformation tensor $\mathbf{F}_E(t)\,(.,t):(n(t))\rightarrow(k(t))$ obtained in such a way is incompatible and should be called the *thermoelastic distortion tensor* whereas $(n(t))$-elements are commonly named as *natural state local reference configurations* (cf. for instance [4, 5]). Of course, the corresponding *plastic distortion tensor* $\mathbf{F}_P\,(.,t):=\mathbf{F}_E\,(.,t)^{-1}\mathbf{F}\,(.,t)$ is not compatible, whereas $\mathbf{F}$ is found by comparison of material fibres in $(k(t_0))$ and $(k(t))$ while $\mathbf{F}_E$ is determined by crystallographic vectors in $(n(t))$ and $(k(t))$([1]). Multiplying the above formula from the left-hand side by $\mathbf{F}_E\,(.,t)$ we reach original Kröner's decomposition rule which is often wrongly named as Lee's decomposition formula.

2˙1. *Micro- and macrorotations of RVE.* – In order to reduce an excessive use of indices and in accord with notation used in classical references like [7] we will use also synonyms $\mathbf{\Phi}\equiv\mathbf{F}_E$ and $\mathbf{\Pi}\equiv\mathbf{F}_P$ to denote elastic and plastic distortions. All these tensors are represented by double tensor fields (cf. [7, 5])

$$\mathbf{F}=F^{k}_{\cdot K}\mathbf{g}_k\otimes\mathbf{g}_0^K,\qquad\mathbf{\Phi}=\Phi^{k}_{\cdot\lambda}\mathbf{g}_k\otimes\mathbf{h}^\lambda,\qquad\mathbf{\Pi}=\Pi^{\lambda}_{\cdot K}\mathbf{h}_\lambda\otimes\mathbf{g}_0^K,\tag{1}$$

where a tacit dependence on *spatial* $\mathbf{g}_k$, *structural* $\mathbf{h}_\kappa$ and *material* $\mathbf{g}_{0K}$ base vectors has been taken into account. Here $\mathrm{d}\mathbf{x}=\mathbf{g}_k\mathrm{d}x^k$, $\mathrm{d}\boldsymbol{\xi}=\mathbf{h}^\lambda\mathrm{d}(\xi)^\lambda$ and $\mathrm{d}\mathbf{x}_0=\mathbf{g}_{0K}\mathrm{d}x_0^K$ and $\mathrm{d}(\xi)^\lambda$ are anholonomic coordinates in the tangent space of $(n(t))$.

Following [3] let us imagine that a typical (n)-element (called in the sequel *representative volume element* and denoted by RVE) is composed of N monocrystal grains, such that each Λ-th grain has N_s slip systems $\mathbf{A}_{\alpha\Lambda}\equiv\mathbf{s}_{\alpha\Lambda}\otimes\mathbf{n}_{\alpha\Lambda},\ \alpha\in\{1,N_s\}$. For instance, for FCC crystals $N_s=12$. Here $\mathbf{s}_{\alpha\Lambda}$ is the unit slip vector and $\mathbf{n}_{\alpha\Lambda}$ is the unit vector normal to the slip plane. For convenience, let us introduce a third unit vector $\mathbf{z}_{\alpha\Lambda}$ normal

([1]) Another more natural approach by Sidoroff and Teodosiu [6] with $\mathbf{F}_P\,(.,t):=\mathbf{F}_E\,(.,t)^{-1}\mathbf{F}\,(.,t)\,\mathbf{F}_E\,(.,t_0)$ is less convenient for further analysis than Kröner's formula. In fact, the only difference is that these authors took into account the initial value of $\mathbf{F}_E\,(.,t)$ comparing $(n(t_0))$ and $(n(t))$ local configurations.

to the considered slip plane (cf. [8,3]) with dyads $\mathbf{A}^1_{\alpha\Lambda} \equiv \mathbf{n}_{\alpha\Lambda} \otimes \mathbf{z}_{\alpha\Lambda}$ and $\mathbf{A}^2_{\alpha\Lambda} \equiv \mathbf{z}_{\alpha\Lambda} \otimes \mathbf{s}_{\alpha\Lambda}$ useful when either cross-slip or climb of dislocations has to be taken into account.

Let structural vectors attached to lattices of grains in the configuration $(n(t))$ be denoted by

$$\mathbf{h}^{\alpha}_{\cdot\,\Lambda}(t) = \mathbf{R}_{\Lambda\Pi}(t)\,\mathbf{h}^{\alpha}(t), \quad \text{where} \quad \alpha \in \{1,3\}, \quad \Lambda \in \{1,N\}. \tag{2}$$

Suppose that a RVE has the volume $\Delta V = \sum_\Lambda \Delta V_\Lambda$. Then introducing grain *concentration* factors $c_\Lambda \equiv \Delta V_\Lambda / \Delta V$ for whole RVE the mean structural vector equals

$$\mathbf{h}^{\alpha}(t) := \sum_{\Lambda} c_\Lambda \mathbf{h}^{\alpha}_{\cdot\,\Lambda}(t). \tag{3}$$

Clearly, the tensors $\mathbf{R}_{\Lambda\Pi}$, $(\Lambda \in \{1,N\})$ describe *relative plastic microrotations* of all grains with respect to the average orientation of the RVE. For monocrystals each of these tensors reduces to unit tensor. Similar formulae hold true for RVE in the initial natural state configuration $(n(t_0))$.

By comparing a RVE in $(n(t))$ and $(n(t_0))$ (cf. fig. 1) we may write a multiplicative formula for the *microplastic distortion tensor*

$$\mathbf{\Pi}_\Lambda := \mathbf{\Pi}_{\Lambda E}\,\mathbf{\Pi}_{\Lambda P}, \tag{4}$$

whose components are the *residual microelastic distortion tensor* $\mathbf{\Pi}_{\Lambda E}$ and *microplastic distortion tensor* $\mathbf{\Pi}_{\Lambda P}$. Having in mind that unit slip vectors satisfy the relationships

$$\mathbf{s}_{\alpha\Lambda}(t) = S^{\alpha}_{\Lambda\beta}\mathbf{h}^{\beta}_{\cdot\,\Lambda}(t), \qquad \mathbf{n}_{\alpha\Lambda}(t) = N^{\alpha}_{\Lambda\beta}\mathbf{h}^{\beta}_{\cdot\,\Lambda}(t), \tag{5}$$

where $S^{\alpha}_{\Lambda\beta} = \text{const}$ and $N^{\alpha}_{\Lambda\beta} = \text{const}$, and assuming that residual microelastic rotation is negligibly small (cf. also [3])([2]) we may finally write

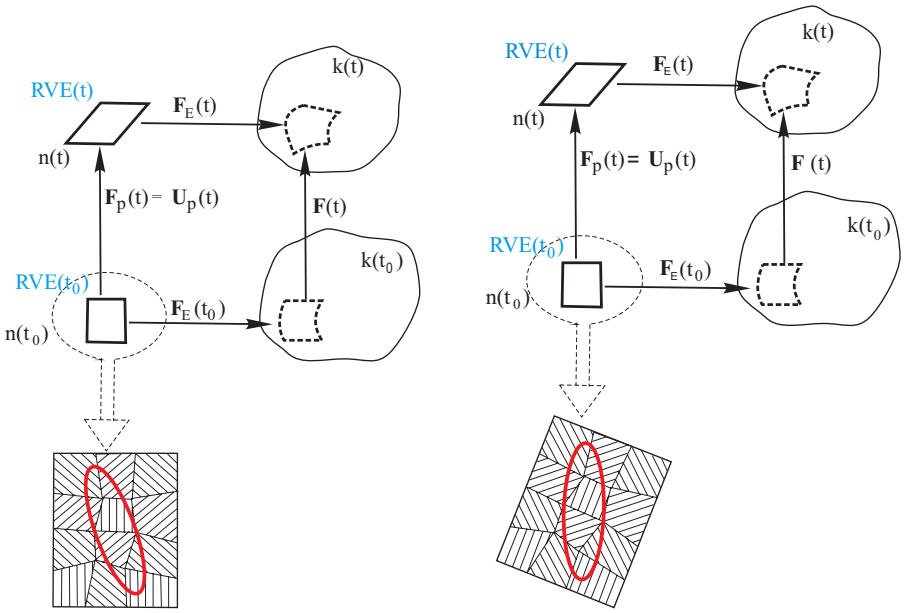
$$\mathbf{\Pi}_\Lambda(t) = \mathbf{V}^{\text{res}}_{\Lambda E}(t)\mathbf{R}_{\Lambda\Pi}(t)\left[\mathbf{1} + \sum_{\alpha} \gamma_{\alpha\Lambda} S^{\alpha}_{\Lambda\beta} N^{\alpha}_{\Lambda\gamma} \mathbf{h}^{\beta}(t) \otimes \mathbf{h}^{\gamma}(t)\right] \mathbf{R}^{T}_{\Lambda\Pi}(t), \tag{6}$$

where $\gamma_{\alpha\Lambda}$ is the slip in the α-th slip system of the Λ-th grain. It is natural to connect here macro- (for RVE) and micro- (for individual grains) plastic distortions by means of spatial averaging $\mathbf{\Pi}(t) = \langle \mathbf{\Pi}_\Lambda(t) \rangle$.

Let us apply the polar decomposition $\mathbf{\Pi} = \mathbf{R}_P \mathbf{U}_P$ to the macroplastic distortion introducing the macroplastic rotation tensor $\mathbf{R}_P$ which is arbitrary (according to Zorawski [9]) and might be fixed either to be a unit tensor or to have Mandel's isoclinicity property (cf. [10] for details). For a definition of isoclinicity we should have to find average crystal directions in $RVE(t)$ and $RVE(t_0)$ and to make them equal. The first choice, *i.e.* $\mathbf{R}_P = \mathbf{1}$ seems more appropriate for polycrystals.

Remark 1 (Plastic rotations). *In this way all the necessary ingredients for a discussion on micro- and macrorotations are prepared. The two mentioned approaches are very useful to fix macroplastic rotations:*

([2]) This does not mean that all the elastic residual rotations are exhausted since macroelastic residual rotation has not been discussed until now.



(a) Average isoclinicity of RVE (average grain orientations parallel)

(b) Macroplastic rotation of RVE fixed (average plastic strain ellipsoids aligned)

Fig. 1. – Rotations of a representative volume element (RVE).

1. *The first way of eliminating macroplastic rotation* $\mathbf{\Pi} = \mathbf{U}_P = \mathbf{C}_P^{1/2}$, *where* $\mathbf{C}_P \equiv \mathbf{\Pi}^T\mathbf{\Pi}$ *greatly simplifies macroplastic spin issue* [10, 3].

2. *The second way could be called Mandel's average macroisoclinicity by the identification:* $\mathbf{h}^\alpha(t) = \mathbf{h}^\alpha(t_0)$, *which approximately aligns plastically deformed RVE in* $(n(t))$ *and* $(n(t_0))$. *For instance, average structural vectors could be aligned to base* $\mathbf{g}_0^K$ *if such an identification is accepted.*

However, for both approaches relative microplastic rotations must not be eliminated unless further tearing of RVE is performed to size of monocrystal grains which is, by assumption, much smaller than the typical dimension of RVE.

At this point it is interesting to note how we can determine macroplastic spin if the macroplastic stretching is known. This issue was discussed in detail in [1]. The above illustrative figure (cf. fig. 1) shows that indeterminate rotation of intermediate local configurations may be fixed either by average isoclinicity or by eliminition of macroplastic rotation of RVE. In both cases plastic spin directly follows from the macroplastic stretching.

Joining RVE in $(n(t))$ into a continuous body requires for each grain microelastic distortion $\mathbf{\Phi}_\Lambda$. Again polar decomposition allows: $\mathbf{\Phi}_\Lambda = \mathbf{R}_{\Lambda E}\mathbf{U}_{\Lambda E}$. Here the right microelastic stretch $\mathbf{U}_{\Lambda E}$ does not include the left microresidual stretch $\mathbf{V}^{\rm res}_{\Lambda E}$. Recalling the "micro-Kröner's" decomposition (4) we could make a new grouping of terms in the following way:

$$\mathbf{F}_\Lambda = \mathbf{R}_{\Lambda E}\ \mathbf{U}_{\Lambda E}\ \mathbf{V}^{\rm res}_{\Lambda E}\ \mathbf{\Pi}_{\Lambda P} \equiv \mathbf{\Phi}_{\Lambda E}\ \mathbf{\Pi}_{\Lambda P}. \tag{7}$$

Here $\mathbf{\Phi}_{\Lambda E}$ encompasses rotation of RVE in $(k(t))$-configuration and residual as well as external forces induced elastic stretches whereas $\mathbf{\Pi}_{\Lambda P}$ includes pure plastic distortion and relative microplastic rotations.

3. – Balance laws

3˙1. *Low-order polycrystals*. – Let us introduce a *mass distribution function* by means of $\varphi(\mathbf{x}') = \{\varphi_\Lambda(\mathbf{x}')|\mathbf{x}' \in \Delta V, \Lambda \in \{1, N\}\}$, with $\varphi_\Lambda(\mathbf{x}') = 1$, $\mathbf{x}' \in \Delta V_\Lambda$ and $= 0$, otherwise.

Then positions of grain centers and RVE-center are determined by

$$\int_{\Delta V} \varphi(\mathbf{x}')\mathbf{x}'\mathrm{d}m' = \mathbf{x}\Delta m, \qquad \int_{\Delta V_\Lambda} \varphi_\Lambda(\mathbf{x}'_0)\mathbf{x}^*_0\mathrm{d}m' = \mathbf{x}^*_{0\Lambda}\Delta m_\Lambda, \tag{8}$$

in the configurations $(k(t))$ and $(k(t_0))$, respectively. Hereinafter the notation $\mathbf{x}' \equiv \mathbf{x}+\mathbf{x}^*$ will be used in the sequel.

Assumption 1. *Suppose that individual grains have the same density and are subject to homogeneous microstrains.*

Such materials are named in [1] as *low-order micromorphic polycrystals*. Moreover, let the center of a RVE be occupied in $(k(t_0))$ and $(k(t))$ by the same material point. According to this assumption deformation gradient is split into its average value and fluctuations as follows: $\mathbf{F}'=\langle\mathbf{F}'\rangle + \mathbf{F}^* \equiv \mathbf{F} + \varphi_\Lambda(\mathbf{x}')\mathbf{F}^*_\Lambda$ (*where* $\mathbf{x}' \in \Delta V_\Lambda$). Let material moments of inertia be

$$\begin{aligned} \mathbf{J}_0 &:= \int_{\Delta V} \varphi(\mathbf{x}'_0)\ \mathbf{x}^*_0 \otimes \mathbf{x}^*_0\ \mathrm{d}m', \\ \mathcal{J}_0 &:= \int_{\Delta V} \varphi(\mathbf{x}'_0)\ \mathbf{x}^*_0 \otimes \mathbf{x}^*_0 \otimes \mathbf{x}^*_0\ \mathrm{d}m', \\ \mathbb{J}_0 &:= \int_{\Delta V} \varphi(\mathbf{x}'_0)\ \mathbf{x}^*_0 \otimes \mathbf{x}^*_0 \otimes \mathbf{x}^*_0 \otimes \mathbf{x}^*_0\ \mathrm{d}m'. \end{aligned} \tag{9}$$

Then momentum, moment of momentum and kinetic energy of such an element read

$$\mathbf{v}\Delta m = \int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\mathrm{d}m' = \dot{\mathbf{x}}\Delta m, \tag{10}$$

$$\Delta\mathbf{l}_O = \int_{\Delta V} \varphi(\mathbf{x}')\mathbf{x}' \times \dot{\mathbf{x}}'\mathrm{d}m' = \left(\mathbf{r} \times \mathbf{v} + \mathcal{E} : \sum_\Lambda c_\Lambda \mathbf{F}_\Lambda \mathbf{J}_{0\Lambda} \dot{\mathbf{F}}^T_\Lambda\right) \Delta m, \tag{11}$$

$$2\Delta T = \int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\dot{\mathbf{x}}'\mathrm{d}m' = \left(\mathbf{v}\mathbf{v} + \sum_\Lambda c_\Lambda \operatorname{tr}\left\{\dot{\mathbf{F}}_\Lambda \mathbf{J}_{0\Lambda} \dot{\mathbf{F}}^T_\Lambda\right\}\right) \Delta m. \tag{12}$$

Consider now stresses and their moments in a RVE. Although Assumption 1 does not require homogeneity of grain distortions but only deformation gradient of a grain inside the considered RVE we will assume that for $\mathbf{x}' \in \Delta V_\Lambda$ their homogeneity

$$\mathbf{\Phi}' = \langle\mathbf{\Phi}'\rangle + \mathbf{\Phi}^* \equiv \mathbf{\Phi} + \varphi_\Lambda(\mathbf{x}')\mathbf{\Phi}^*_\Lambda, \qquad \mathbf{\Pi}' = \langle\mathbf{\Pi}'\rangle + \mathbf{\Pi}^* \equiv \mathbf{\Pi} + \varphi_\Lambda(\mathbf{x}')\mathbf{\Pi}^*_\Lambda \tag{13}$$

also holds. At $\mathbf{x}' \in \Delta V_\Lambda$ let the second Piola-Kirchhoff ($(n(t))$-related) and Cauchy stress be related by means of $\mathbf{\Phi}'\mathbf{S}'\mathbf{\Phi}'^T = \mathbf{T}' \det \mathbf{\Phi}'$.

The vector of stress moments for RVE is given by

$$\Delta\mathbf{m}_O = \int_{\partial\Delta V} \varphi(\mathbf{x}')\mathbf{x}' \times \mathbf{T}'\mathbf{n}' \mathrm{d}s' = \int_{\Delta V} \varphi(\mathbf{x}') \operatorname{div}(\mathbf{x}' \times \mathbf{T}') \mathrm{d}V' = \Delta V(\mathbf{x} \times \operatorname{div}\mathbf{T} - \boldsymbol{\tau}) + \sum_\Lambda \Delta S_\Lambda (\mathbf{x}^* \times [[\mathbf{T}^*_\Lambda]]\ \mathbf{n}_\Lambda)|_{\partial\Delta V_\Lambda}. \tag{14}$$

Here again we have splitting $\mathbf{T}' = \langle \mathbf{T}' \rangle + \mathbf{T}^* = \mathbf{T} + \varphi_\Lambda(\mathbf{x}')\mathbf{T}^*_\Lambda$ for $\mathbf{x}' \in \Delta V_\Lambda$ whereas $[[\mathbf{T}^*_\Lambda]]$ denotes jump of the fluctuation of Cauchy stress on boundaries of Λ-th grain (cf. also [11]). The average Cauchy stress is here divided into its antysymmetric and symmetric parts by means of

$$\boldsymbol{\tau} = \frac{1}{2}\mathcal{E} : \mathbf{T}, \qquad \mathbf{T}_\mathbf{a} = \mathcal{E}\boldsymbol{\tau} \equiv \frac{1}{2}(\mathbf{T} - \mathbf{T}^T), \qquad \mathbf{T}_s = \frac{1}{2}(\mathbf{T} + \mathbf{T}^T) \equiv \boldsymbol{\sigma}. \tag{15}$$

In the same way the mechanical working done by microstresses throughout RVE equals

$$\Delta P = \int_{\partial\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\mathbf{T}'\mathbf{n}' \mathrm{d}s' = \sum_\Lambda \Delta S_\Lambda (\mathbf{x}^* \times [[\mathbf{T}^*_\Lambda]]\ \mathbf{n}_\Lambda)|_{\partial\Delta V_\Lambda} + \Delta V \left(\mathbf{T} : \operatorname{grad}\dot{\mathbf{x}} + \dot{\mathbf{x}} \operatorname{div}\mathbf{T} + \sum_\Lambda c_\Lambda \mathbf{T}^*_\Lambda : \operatorname{grad}\dot{\mathbf{x}}^*_\Lambda \right). \tag{16}$$

Now we are ready to write balance equations for typical RVE. First, balance of momentum leads to the traditional nonpolar equation, *i.e.* $\rho\ddot{\mathbf{x}} = \operatorname{div}\mathbf{T}$ (cf. [1]), whereas balance of moment of momentum $D\Delta\mathbf{l}_O/Dt = \Delta\mathbf{m}_O$ gives the antysymmetric part of Cauchy stress([3]) as follows([4]):

$$2\boldsymbol{\tau} = -\rho\mathcal{E} : \sum_\Lambda c_\Lambda \mathbf{F}_\Lambda \mathbf{J}_\Lambda \ddot{\mathbf{F}}^T_\Lambda + \frac{1}{\Delta V} \sum_\Lambda \Delta S_\Lambda (\mathbf{x}^* \times [[\mathbf{T}^*_\Lambda]]\ \mathbf{n}_\Lambda)|_{\partial\Delta V_\Lambda}. \tag{17}$$

The last balance law is the first law of thermodynamics which for the RVE reads

$$\Delta\dot{T} + \Delta\dot{E} = \Delta P + \Delta Q, \tag{18}$$

where $\Delta\dot{E}$ is the time rate of internal energy, while ΔP and ΔQ are mechanical and nonmechanical working which includes thermal effects. If the average velocity gradient

---

([3]) From (17) we see that for low-order micromorphic polycrystals stress is symmetric only if the two following conditions are satisfied: a) intergranular continuity which means that stress vector is continuous on grain boundaries and b) proportional paths meaning that deformation gradient of each grain follows a proportional path. The second condition is approximately satisfied also when *higher-order inertial terms* (*i.e.* first sum on RHS of the above equation) are negligibly small.

([4]) The integrals in this and subsequent relationships do not appear since our attention is focused to the low-order micromorphic inelastic polycrystals [1].

tensor $\mathbf{L} \equiv \operatorname{grad} \dot{\mathbf{x}}$ is split into its symmetric and antysymmetric parts,

$$\boldsymbol{\omega} = \frac{1}{2}\mathcal{E} : \mathbf{L}, \qquad \mathbf{L_a} = \mathcal{E}\boldsymbol{\omega} \equiv \frac{1}{2}(\mathbf{L} - \mathbf{L^T}), \qquad \mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T) \equiv \mathbf{L}_s, \tag{19}$$

then the energy conservation law may be written in the following way:

$$\begin{aligned} \rho\, \dot{e} - \boldsymbol{\sigma} : \mathbf{D} = 2\boldsymbol{\tau}\boldsymbol{\omega} - \frac{1}{2}\rho \sum_{\Lambda} c_\Lambda \operatorname{tr}\left\{ \ddot{\mathbf{F}}_\Lambda \mathbf{J}_\Lambda \dot{\mathbf{F}}_\Lambda^T + \dot{\mathbf{F}}_\Lambda \mathbf{J}_\Lambda \ddot{\mathbf{F}}_\Lambda^T \right\} \\ + \sum_{\Lambda} c_\Lambda (\boldsymbol{\sigma}_\Lambda^* : \mathbf{D}_\Lambda^* + 2\boldsymbol{\tau}_\Lambda^* \boldsymbol{\omega}_\Lambda^*) + \frac{1}{\Delta V} \sum_{\Lambda} \Delta S_\Lambda (\dot{\mathbf{x}}^* [[\mathbf{T}_\Lambda^*]]\ \mathbf{n}_\Lambda)|_{\partial \Delta V_\Lambda}. \end{aligned} \tag{20}$$

3˙2. *A comment on homogenization.* – Let us describe now approximately grain behaviour by some smooth functions. Following [12], the easiest way to do that is to suppose that deformation gradient and distortions are linear functions of position throughout the considered RVE, *i.e.*

$$\bar{\mathbf{F}}' = \bar{\mathbf{F}} + \mathcal{F}\mathbf{x}_0^*, \qquad \bar{\boldsymbol{\Phi}}' = \bar{\boldsymbol{\Phi}} + \mathbf{x}^* \mathcal{F}_E, \qquad \bar{\boldsymbol{\Pi}}' = \bar{\boldsymbol{\Pi}} + \mathcal{F}_P \mathbf{x}_0^* \tag{21}$$

(cf. also (8)). Now, the approximating "constants" $\bar{\mathbf{F}}$ and $\mathcal{F}$ are found by minimization of the functional

$$I = \frac{1}{\Delta V} \int_{\Delta V} \|\bar{\mathbf{F}}' - \mathbf{F}'\|^2 \mathrm{d}V' \qquad \Longrightarrow \qquad \min_{(\bar{\mathbf{F}}, \mathcal{F})} I \Rightarrow (\bar{\mathbf{F}}, \mathcal{F}), \tag{22}$$

which means that I has the role of the so-called chi-square function.

Taking the inner product as a means to form the above norm we get linear approximations for total deformation and distortions([5]):

$$\begin{aligned} \bar{\mathbf{F}} &= \mathbf{F} \quad \text{as well as} \quad \mathcal{F} = \langle \mathbf{F}^* \otimes \mathbf{x}_0^* \rangle \langle \mathbf{J}_0 \rangle^{-1}, \\ \bar{\boldsymbol{\Pi}} &= \boldsymbol{\Pi} \quad \text{as well as} \quad \mathcal{F}_P = \langle \boldsymbol{\Pi}^* \otimes \mathbf{x}_0^* \rangle \langle \mathbf{J}_0 \rangle^{-1}, \\ \bar{\boldsymbol{\Phi}} &= \boldsymbol{\Phi} \quad \text{as well as} \quad \mathcal{F}_E = \langle \mathbf{J} \rangle^{-1} \langle \mathbf{x}^* \otimes \boldsymbol{\Phi}^* \rangle, \end{aligned} \tag{23}$$

where the *spatial grain microinertia tensor* has the following form (cf. also (9)):

$$\mathbf{J} := \int_{\Delta V} \varphi(\mathbf{x}')\ \mathbf{x}^* \otimes \mathbf{x}^*\ \mathrm{d}m'.$$

Remark 2 (Dislocation densities). *Antysymmetric parts of $\mathcal{F}_E$ and $\mathcal{F}_P$ are third-order true spatial and material dislocation density tensors (cf.* [13, 14, 5]*):*

$$\mathbf{A}_E = \mathcal{E} : \mathcal{F}_E, \qquad \mathbf{A}_P = \mathcal{F}_P : \mathcal{E}_0, \tag{24}$$

where the two Ricci permutation tensors in spatial and material coordinates are given by: $\mathcal{E} = \mathcal{E}_{abc}\mathbf{g}^a \otimes \mathbf{g}^b \otimes \mathbf{g}^c$ and $\mathcal{E}_0 = \mathcal{E}_{KLM}\mathbf{g}_0^K \otimes \mathbf{g}_0^L \otimes \mathbf{g}_0^M$, respectively. The two representations

([5]) Although we apply the same type of approximation functions for $\mathbf{F}'$ and $\boldsymbol{\Phi}'$, $\boldsymbol{\Pi}'$ it would be possible to have $\mathcal{F} = 0$, but $\mathcal{F}_P \neq 0$, $\mathcal{F}_E \neq 0$ for instance.

of dislocation density are connected by: $\mathbf{A}_E \det \mathbf{\Phi} = \mathbf{A}_P \mathbf{F}^T$. *It must be noted that early papers of Kondo, Bilby, Kröner, Stojanović and their collaborators on non-Euclidean geometry of natural state space are so pregnant that the subject would require a separate analysis. Of special interest is here non-Euclidean geometry of oriented materials like Cosserat media. A lot of other important remarks about non-Euclidean aspects of geometry of deformation could be made (cf., e.g.,* [5]*) but have to be omitted for the sake of brevity.*

For further analysis of constitutive equations we will need balance laws for such a linearly smoothed RVE. The balance equation for momentum is unchanged. On the other hand, the moment of momentum becomes (with a synonymous $\mathrm{D}\mathcal{F}/\mathrm{D}t \equiv \mathcal{F}_t$):

$$
\begin{aligned}
(25) \qquad 2\boldsymbol{\tau}\Delta V = \sum_{\Lambda} \int_{\partial \Delta V_\Lambda} (\mathbf{x}^* \times [[\mathbf{T}^*_\Lambda]]\ \mathbf{n}_\Lambda) \mathrm{d}S'_\Lambda - \rho\mathcal{E} : (\mathbf{F}\mathbf{J}_0\ddot{\mathbf{F}}^T + \mathcal{F} : \mathbb{J}_0 : \mathcal{F}^T_{tt}) \\
-\rho\mathcal{E} : \frac{\mathrm{D}}{\mathrm{D}t}(\mathbf{F}\mathcal{J}_0 : \mathcal{F}^T_t + \mathcal{F} : \mathcal{J}_0\dot{\mathbf{F}}^T),
\end{aligned}
$$

where higher-order material inertia moments are given above by (9) (cf. also [15]). Bar above F is missing due to homogenization (23).

To derive the energy balance equation, let us start with the expression for kinetic energy of RVE:

$$
\begin{aligned}
(26) \qquad 2\frac{\Delta T}{\Delta m} = \frac{1}{\Delta m}\int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\dot{\mathbf{x}}' \mathrm{d}V' = \mathbf{v}\mathbf{v} + \mathrm{tr}(\dot{\mathbf{F}}\mathbf{J}_0\dot{\mathbf{F}}^T) \\
+ \mathrm{tr}(\dot{\mathbf{F}}\mathcal{J}_0 : \mathcal{F}^T_t + \mathcal{F}_t : \mathcal{J}_0\dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}^T_t).
\end{aligned}
$$

In order to obtain an expression for mechanical working, we suppose that velocity gradient $\mathbf{L}'$ is also a linear function throughout a RVE:

$$
(27) \qquad \mathbf{D}' = \mathbf{D} + \mathbf{x}^* \operatorname{grad}\mathbf{D}, \qquad \boldsymbol{\omega}' = \boldsymbol{\omega} + \mathbf{x}^* \operatorname{grad}\boldsymbol{\omega},
$$

such that (with notation $\mathcal{A} \circ \mathcal{B} = \mathcal{A}^{abc}\mathcal{B}_{abc}$)

$$
\begin{aligned}
(28) \qquad \frac{\Delta P}{\Delta V} - \dot{\mathbf{x}} \operatorname{div}\mathbf{T} - \boldsymbol{\sigma} : \mathbf{D} = 2\boldsymbol{\tau}\boldsymbol{\omega} + \mathcal{M} \circ \operatorname{grad}\mathbf{D} + 2\mathbf{M} : \operatorname{grad}\boldsymbol{\omega} \\
+ \frac{1}{\Delta V}\sum_{\Lambda} \int_{\partial \Delta V_\Lambda} (\dot{\mathbf{x}}\ [[\mathbf{T}^*_\Lambda]]\ \mathbf{n}_\Lambda) \mathrm{d}S'_\Lambda,
\end{aligned}
$$

where moments of the symmetric and antysymmetric stress are

$$
(29) \qquad \mathcal{M}\ \Delta V = \int_{\Delta V} \boldsymbol{\sigma}^* \otimes \mathbf{x}^*\, \mathrm{d}V', \qquad \mathbf{M}\ \Delta V = \int^*_{\Delta V} \boldsymbol{\tau}^* \otimes \mathbf{x}^*\, \mathrm{d}V',
$$

respectively, and vanish in the case of homogeneous stress state inside a RVE. Finally, by means of relations (26) and (28) energy conservation equation (18) for RVE obtains

the following form (the average heat flux vector is denoted by $\mathbf{q}$, *i.e.* $\mathbf{q} = \langle \mathbf{q}' \rangle$):

$$
\begin{aligned}
(30) \qquad \rho\, \dot{e} - \boldsymbol{\sigma} : \mathbf{D} - \operatorname{div} \mathbf{q} = \rho \frac{\mathrm{D}}{\mathrm{D}t} \operatorname{tr}(\dot{\mathbf{F}} \mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F}_t : \mathcal{J}_0 \dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}_t^T) \\
+ 2\boldsymbol{\tau}\boldsymbol{\omega} + \mathcal{M} \circ \operatorname{grad} \mathbf{D} + 2\mathbf{M} : \operatorname{grad} \boldsymbol{\omega} + \rho \frac{\mathrm{D}}{\mathrm{D}t}\ \operatorname{tr}\{\dot{\mathbf{F}} \mathbf{J}_0 \dot{\mathbf{F}}^T\} \\
+ \frac{1}{\Delta V} \sum_{\Lambda} \int_{\partial \Delta V_\Lambda} (\dot{\mathbf{x}}\ [[\mathbf{T}^*]]\ \mathbf{n}) \mathrm{d}S'_\Lambda .
\end{aligned}
$$

4. – Evolution and constitutive equations

4˙1. *Constitutive equations for stress and its moment.* – For the analysis in this section it is useful to express the energy equation (30) in terms of intermediate local reference configuration. Moreover let us suppose that Condition 1 is fulfilled, *i.e.* that stress vector is continuous on grain boundaries.

Recalling the definition of $\mathbf{S}'$ we denote its symmetric and antysymmetric parts by $\boldsymbol{\sigma}'_S$ and $\boldsymbol{\tau}'_S$, while elastic stretching is nothing but $\dot{\mathbf{E}}'_E$ and the antysymmetric part of the elastic "velocity gradient", denoted by $\mathbf{L}'_E := \dot{\boldsymbol{\Phi}}'(\boldsymbol{\Phi}')^{-1}$, is given by the vector $\boldsymbol{\omega}'_E$. Then the energy conservation equation may be transformed to

$$
\begin{aligned}
(31) \qquad \rho_0\, \dot{e} - \operatorname{Div} \mathbf{q}_{(n)} = \rho_0 \frac{\mathrm{D}}{\mathrm{D}t} \operatorname{tr}(\dot{\mathbf{F}} \mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F}_t : \mathcal{J}_0 \dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}_t^T) \\
+ \boldsymbol{\sigma}_S : \dot{\mathbf{E}}_E + \mathcal{M}_S \circ \operatorname{Grad} \dot{\mathbf{E}}_E + 2\boldsymbol{\tau}_S \boldsymbol{\omega}_E + 2\mathbf{M}_S : \operatorname{Grad} \boldsymbol{\omega}_E \\
+ \rho_0 \frac{\mathrm{D}}{\mathrm{D}t}\ \operatorname{tr}\{\dot{\mathbf{F}} \mathbf{J}_0 \dot{\mathbf{F}}^T\} + R(\dot{\boldsymbol{\Pi}}, \operatorname{Grad} \dot{\boldsymbol{\Pi}}),
\end{aligned}
$$

where the last term on RHS is linear in material time rates of plastic distortion and plastic distortion gradient tensors whereas

$$
\mathbf{q}_{(n)} = \left\langle (\boldsymbol{\Phi}')^{-1} \mathbf{q}' \det \boldsymbol{\Phi}' \right\rangle
$$

is the average heat flux vector related to $(n(t))$, $\operatorname{Grad}(\bullet) := \boldsymbol{\Phi} \operatorname{grad}(\bullet)$, $\rho_0 = \rho \det \boldsymbol{\Phi}$ and

$$
(32) \qquad \mathcal{M}_S\ \Delta V_0 = \int_{\Delta V} \boldsymbol{\sigma}^*_S \otimes \boldsymbol{\xi}^*\ \mathrm{d}V'_0, \qquad \mathbf{M}_S\ \Delta V_0 = \int_{\Delta V}^{*} \boldsymbol{\tau}^*_S \otimes \boldsymbol{\xi}^*\ \mathrm{d}V'_0 .
$$

We want to exploit the above energy equation in order to get some constitutive restrictions for stresses and their moments. First the internal energy function must be analyzed in order to see on which arguments it depends. Let us start with Hooke's law for each grain and compose them into RVE. For an arbitrary point inside RVE we obtain by means of Hooke's law for each grain the following expression:

$$
(33) \qquad 2e' = \mathbf{E}'_E : \mathbb{D}' : \mathbf{E}'_E = (\mathbf{E}_E + \mathbf{E}^*_E) : (\mathbb{D} + \mathbb{D}^*) : (\mathbf{E}_E + \mathbf{E}^*_E),
$$

where $\mathbb{D}' = \mathbb{R}'_\Pi : \mathbb{D}_0 : \mathbb{R}'^T_\Pi = \varphi_\Lambda(\mathbf{x}')\mathbb{D}_\Lambda$ depends again on grain orientations while the average elastic strain $2\mathbf{E}_E = \boldsymbol{\Phi}^T\boldsymbol{\Phi} - \mathbf{1}_n$ follows from the homogenization (23). The spatial

averaging of the above relationship leads to

$$2e = 2e_{HM} + (\mathbf{J}_{(n)}\,\mathrm{Grad}\,\mathbf{E}_E : \mathbb{D}_0^T) \circ \mathrm{Grad}\,\mathbf{E}_E + \mathbf{E}_E : \langle \mathbb{D}^* \otimes \boldsymbol{\xi}^* \rangle \circ (\mathrm{Grad}\,\mathbf{E}_E)^T + \mathrm{Grad}\,\mathbf{E}_E \circ \langle \boldsymbol{\xi}^* \otimes \mathbb{D}^* \rangle : \mathbf{E}_E + \mathrm{Grad}\,\mathbf{E}_E \circ \langle \boldsymbol{\xi}^* \otimes \mathbb{D}^* \otimes \boldsymbol{\xi}^* \rangle \circ (\mathrm{Grad}\,\mathbf{E}_E)^T \tag{34}$$

with notations $\mathbf{J}_{(n)} \equiv \langle \boldsymbol{\xi}^* \otimes \boldsymbol{\xi}^* \rangle$ and $(\mathrm{Grad}\,\mathbf{E}_E)^T_{\lambda\alpha\beta} = (\mathrm{Grad}\,\mathbf{E}_E)_{\alpha\beta\lambda}$. Here by $2e_{HM} = \mathbf{E}_E : \mathbb{D}_0 : \mathbf{E}_E$ we denote the Hill-Mandel approximation of our internal energy function [11]. It is worthy of note that the above expression contains also third-order products (cf. last term on RHS).

Suppose that inertial higher-order terms in (34) are negligible. The differentiation of the above internal energy function and its replacement into (31) leads to constitutive restrictions for the symmetric part of the stress tensor and its moment as follows:

$$\frac{1}{\rho_0}\boldsymbol{\sigma}_S = \frac{\partial e}{\partial \mathbf{E}_E} = \mathbb{D}_0 : \mathbf{E}_E + \langle \mathbb{D}^* \otimes \boldsymbol{\xi}^* \rangle \circ (\mathrm{Grad}\,\mathbf{E}_E)^T, \tag{35a}$$

$$\frac{1}{\rho_0}\mathcal{M}_S = \frac{\partial e}{\partial\, \mathrm{Grad}\,\mathbf{E}_E} = \mathbf{J}_{(n)}\,\mathrm{Grad}\,\mathbf{E}_E : \mathbb{D}_0^T + \langle \boldsymbol{\xi}^* \otimes \mathbb{D}^* \rangle : \mathbf{E}_E + \langle \boldsymbol{\xi}^* \otimes \mathbb{D}^* \otimes \boldsymbol{\xi}^* \rangle \circ (\mathrm{Grad}\,\mathbf{E}_E)^T. \tag{35b}$$

The following special case of the above constitutive relations is of special interest to us.

Remark 3 (Isotropic grains). *Suppose that each grain is elastically isotropic which means* $\mathbb{D}' = \mathbb{D}_0(\lambda, \mu)$*, or, equivalently,* $\mathbb{D}^* = 0$*. Then*

$$2e = \lambda(\mathrm{tr}\,\mathbf{E}_E)^2 + 2\mu\ \mathrm{tr}(\mathbf{E}_E^2) + \lambda \mathbf{J}_{(n)} : [\mathrm{Grad}(\mathrm{tr}\,\mathbf{E}_E) \otimes \mathrm{Grad}(\mathrm{tr}\,\mathbf{E}_E)] + 2\mu(\mathbf{J}_{(n)}\,\mathrm{Grad}\,\mathbf{E}_E) \circ \mathrm{Grad}\,\mathbf{E}_E.$$

The main advantage of this expression is that it does not need any new material constant. The microinertia tensor may be calculated explicitly and in the special case when tessellation of RVE into grains is by means of cubes we would have its diagonal terms equal to $1/12$ *whereas its off-diagonal terms would be* $1/16$*. For instance, in the paper of Lubarda and Markenscoff (cf.* [16] *formula* (42)*) they have one additional constant and an unknown scaling length. As another example, Fleck and Hutchinson in* [17] *have five additional material constants and apply the so-called* J_2*-theory in discussing their influence on the overall inelastic behaviour of RVE.*

4˙2. *Evolution equation.* – According to the principle of inelastic memory introduced in [10] the second Piola-Kirchhoff stress is given by a very general functional accounting for plastic strain as well as plastic strain rate history, where the macroplastic strain tensor could be for instance $\boldsymbol{\varepsilon}_P = \mathbf{U}_P - \mathbf{1}$ (cf. Remark 1). When such a functional may be transformed into a nonlinear function of plastic strain and plastic strain rate the plastic material is of *differential type* (cf. [10]). Solving such an equation in plastic strain rate we would obtain the following evolution equation:

$$\dot{\boldsymbol{\varepsilon}}_P = \dot{\boldsymbol{\varepsilon}}_P(\mathbf{S}, \boldsymbol{\varepsilon}_P) \tag{36}$$

which, by means of tensor representation theory [18, 19, 10], can be explicitly written as follows:

$$\dot{\mathbf{U}}_P = \langle f\rangle[d_1(\chi)\mathbf{1} + d_2(\chi)\mathbf{U}_P + d_3(\chi)\mathbf{U}_P^2 + d_4(\chi)\mathbf{S} + d_5(\chi)\mathbf{S}^2 + d_6(\chi)(\mathbf{S}\mathbf{U}_P + \mathbf{U}_P\mathbf{S}) + d_7(\chi)(\mathbf{S}^2\mathbf{U}_P + \mathbf{U}_P\mathbf{S}^2) + d_8(\chi)(\mathbf{S}\mathbf{U}_P^2 + \mathbf{U}_P^2\mathbf{S})], \tag{37}$$

where the bracket $\langle f\rangle = 1$ if plastic deformation takes place and $\langle f\rangle = 0$ otherwise. Suppose that the assumption of absence of macroplastic rotations holds (cf. Remark 1). Then from the expression for macroplastic stretching there follows a relationship for macroplastic spin without any new material constants [1]. Such a conclusion may be also derived for average macroisoclinicity (cf. [10] for details) but the procedure is much more tedious.

For the time being let us restrict our attention to the nonpolar case when stress is symmetric. After [20] from the plastic power (which is not a time derivative since it depends on trajectory):

$$P_t^{\mathrm{in}} := \mathbf{T} : \mathbf{D} - \mathbf{S} : \dot{\mathbf{E}}_E = \frac{1}{2}\mathbf{S} : (\mathbf{C}_E\dot{\mathbf{U}}_P\mathbf{U}_P^{-1} + \mathbf{C}_E\mathbf{U}_P^{-1}\dot{\mathbf{U}}_P) \equiv \mathbf{S}_U : \dot{\mathbf{U}}_P, \tag{38}$$

we define the isotropic hardening parameter p as the integral $p(t) = \int_0^t P_t^{\mathrm{in}}(\tau)\mathrm{d}\tau$. Then, following [21] we take the specific free energy g of the considered body in the form

$$g = g_E(\mathbf{E}_E, T) + g_P(p, T). \tag{39}$$

Now, by means of the second law of thermodynamics we have $\aleph \equiv \rho\,\dot{s} + \mathrm{div}(\mathbf{q}/T) \geq 0$, where T is the absolute temperature and s the specific entropy. Since the free energy is assumed in the form (39) the dissipation is determined by means of the following expression: $T\aleph = (1 - \rho\partial_p g)P_t^{\mathrm{in}}$. By making use of this dissipation Vakulenko introduced a concept of *thermodynamic time* by the following hereditary function (cf. [22]):

$$\zeta(t) := \int_0^t \psi[T\aleph(\tau)]\,\mathrm{d}\tau. \tag{40}$$

The function $\zeta(t)$ is piecewise continuous and nondecreasing in the way that $\dot{\zeta}(t) = 0$ within elastic ranges and $\dot{\zeta}(t) > 0$ when plastic deformation takes place. Splitting the whole time history into a sequence of infinitesimal segments Vakulenko claimed that a superposition and causality exists such that the plastic strain tensor is a functional of stress and stress rate history such that

$$\boldsymbol{\varepsilon}_P(\zeta) = \int_0^{\zeta} \boldsymbol{\Psi}[\zeta - \xi, \mathbf{S}(\xi), \dot{\mathbf{S}}(\xi), p(\xi)]\,\mathrm{d}\xi. \tag{41}$$

In [3] the accumulated plastic strain $\pi(\zeta) \equiv \int_0^{\zeta} \|\dot{\boldsymbol{\varepsilon}}_P(\xi)\|\mathrm{d}\xi$ is added extending in such a way Vakulenko's arguments. Of course, this integral equation is adopted to our case of finite macroplastic strains and absence of macroplastic rotation. Differentiation of (41) with respect to the thermodynamic time gives

$$\partial_\zeta\boldsymbol{\varepsilon}_P = \boldsymbol{\Psi}[0, \mathbf{S}(\zeta), \dot{\mathbf{S}}(\zeta), \pi(\zeta)] + \int_0^{\zeta} \partial_\zeta\boldsymbol{\Psi}[\zeta - \xi, \mathbf{S}(\xi), \dot{\mathbf{S}}(\xi), \pi(\xi)]\,\mathrm{d}\xi. \tag{42}$$

When the tensorial kernel in (41) is chosen in such a way that

$$\boldsymbol{\Psi}[\zeta-\xi,\mathbf{S}(\xi),\dot{\mathbf{S}}(\xi),\pi(\xi)] = J(\zeta-\xi)\;\partial_\xi\sigma_{\mathrm{eq}}(\xi)\boldsymbol{\Psi}_1(\mathbf{S}(\xi),\pi(\xi)) + \boldsymbol{\Psi}_2(\mathbf{S}(\xi),\pi(\xi)) \tag{43}$$

and $\partial_\zeta\, J(\zeta-\xi)=0$, then the integral on the right-hand side of (42) vanishes. If, moreover, the function in (40) is of the power type, *i.e.* $\psi[T\aleph]=(T\aleph)^a$, then a multiplication of (42) by $\dot\zeta$ transforms this equation into

$$\dot{\mathbf{U}}_P = \boldsymbol{\Psi}_1 J(0)\,\dot\sigma_{\mathrm{eq}} + \boldsymbol{\Psi}_2\dot\zeta. \tag{44}$$

Its multiplication by $\mathbf{S}_U$ allows further $P_t^{\mathrm{in}} = i_1 J(0)\,\dot\sigma_{\mathrm{eq}} + i_2(1-\rho\partial_p f)^a (P_t^{\mathrm{in}})^a$, where $i_\alpha = \mathbf{S}_U : \boldsymbol{\Psi}_\alpha$, $\alpha\in\{1,2\}$. The explicit solution of this equation, *i.e.* $P_t^{\mathrm{in}} = P_t^{\mathrm{in}}(\dot\sigma_{\mathrm{eq}}, i_1, i_2)$ depends on the value of the exponent a. If value $a=1$ suggested in [22] is taken, then the correction introduced by means of the tensor $\boldsymbol{\Psi}_2$ seems unnecessary apart from the stress rate-dependent kernel $J(\zeta-\xi)$ (cf. (45)). However, for $a<1$ we have *decelarated ageing* whereas $a>1$ would define *accelarated ageing* [20]. Vakulenko's value $a=1$ might be termed as *steady ageing*. Nonsteady ageing has the advantage to explain also creep-plasticity interaction [3].

4˙3. *Nonpolar case by loading function normality and experiments.* – If $\boldsymbol{\Psi}_2$ is negligibly small, then evolution equation (42) looks like incremental. The corresponding reduced evolution equation $\dot{\mathbf{U}}_P = \boldsymbol{\Psi}_1 J(0)\,\dot\sigma_{\mathrm{eq}}$ belongs to the class of hereditary equations with thermodynamic time as introduced by Vakulenko. However, the experiments, described in [20], have shown that equivalent plastic strain rate and equivalent stress rate are approximately proportional. Then the integral equation with a kernel J is the logical outcome:

$$\pi(t) = \int_0^t J(t-t')\;\dot\sigma_{\mathrm{eq}}(t')\;\mathrm{d}t', \qquad \text{with} \qquad J(t-\tau) = \begin{cases} 0, & \tau\geq t^*,\\ \exp[-M], & \tau<t^*. \end{cases} \tag{45}$$

Here t^* is used to denote instant of onset of plastic straining which happens when the equivalent stress reaches the critical stress rate-dependent initial yield stress $Y_0(\dot\sigma_{\mathrm{eq}})$, such that $\sigma_{\mathrm{eq}}(t^*) = Y_0[\dot\sigma_{\mathrm{eq}}(t^*)]$. At first sight the evolution equation for plastic stretching seems rate independent since it can be transformed into an incremental equation if it is multiplied by an infinitesimal time increment. However, the rate dependence appears in the trigger stress rate-dependent value of the initial yield stress.

Concerning the tensor function $\boldsymbol{\Psi}_1$ it can either have the form (37) or it could be determined by an orthogonality of plastic stretching onto a yield function. Taking such a function to be a third-rank polynomial tensor function of stress we obtain the MAM reduced model (cf. [20], Chapter 5)([6])

$$2\Omega = a_1 s_2 + a_2(s_1 s_2 - s_3). \tag{46}$$

Applying Rice's reasoning [23, 24], *i.e.* we arrive at the result

$$\frac{1}{\Lambda}\mathbf{D}_P = \frac{\partial\Omega}{\partial\mathbf{S}} = (a_1+a_2 s_1)\mathbf{S}_d/Y_0 - 3/2 a_2(\mathbf{S}_d^2)_d, \qquad \text{with} \qquad \Lambda = J(0)\,\dot\sigma_{\mathrm{eq}}\,\pi^\beta, \tag{47}$$

([6]) As shown in [20] this is the simplest nonlinear evolution equation for plastic stretching.

where: $s_\alpha \equiv \mathrm{tr}(\mathbf{S}^\alpha), \alpha \in \{1,2,3\}$—the stress invariants, $\dot{\pi} = \|\mathbf{D}_P\|$—the so-called *equivalent plastic strain rate* and $\mathbf{S}_d$ is the deviatoric part of the Piola-Kirchhoff stress $\mathbf{S}$, while $\sigma_{\mathrm{eq}} \equiv \|\mathbf{S}_d\|$ denotes the *equivalent Mises stress*. We note here that the above equation is a special case of (37). A special attention deserves the assumed normality (47) and a detailed discussion on it as well as on nonlocality is given in [3] criticizing the normality assumption. Anyway, the very simple equation (47) with just three material constants, namely, a_1, a_2, β and one "*universal constant*" M [25] showed very high agreement with multiaxial experiments from very low ($D\pi \sim 0.001\,\mathrm{s}^{-1}$) to very high strain rates ($D\pi \sim 1000\,\mathrm{s}^{-1}$) for diverse specimens: the uniaxial tension with cylindrical specimen, shear by "bicchierino" specimen and cruciform specimen. The wording universal (especially chosen to confront with the so-called universal flow rule appearing in J_2 theories) means that it covers all types of tests for a single material. Of course, this is just a material constant. However using it the necessary number of material constants is drastically reduced as compared with other viscoplasticity theories.

4˙4. *Evolution equations—polar case*. – In the paper [26] the authors assumed that their yield function depends also on the magnitude of the equivalent stress gradient: $\|\operatorname{grad}(\sigma_{\mathrm{eq}})\|$.

On the other hand, in a well-known paper [24], Rice introduced the notion of "*pattern of internal rearrangement*" (PIR) stating that: "any local microstructural rearrangement within the material is dependent on the current stress state only through the thermodynamic force conjugate to the extent of that rearrangement". This approach then leads to plastic power where, like in the case of Onsager relations, he obtained normality by flow potential (or loading function). The associated generalized velocity and associated force are plastic stretching and force. Thus, $\mathbf{D}_P = \partial\Omega/\partial\mathbf{S}$ is obtained. We would like to extend this PIR approach to polar case by a very simple extension of the loading function:

$$\Omega = \hat{\Omega}(s_\alpha, \operatorname{grad} s_\alpha). \tag{48}$$

As known from the theory of invariants (*e.g.* [19]), the characteristic invariants for vectors are

$$s_{\alpha\beta} = \operatorname{grad} s_\alpha \operatorname{grad} s_\beta, \quad \alpha,\beta \in \{1,2,3\}. \tag{49}$$

Before applying generalized normality in the spirit of Rice's theory of PIR, let us repeat formulae for linear approximation of plastic stretching and stress within the RVE (cf. (27)):

$$\mathbf{D}'_P = \mathbf{D}_P + \mathbf{x}^* \operatorname{grad}\mathbf{D}_P, \qquad \mathbf{S}' = \mathbf{S} + \mathbf{x}^* \operatorname{grad}\mathbf{S}, \tag{50}$$

where again position vectors $\mathbf{x}^*$ are taken from the center of the RVE. Then, neglecting elastic strains in (38) and applying (50) to it we arrive at

$$P_t^{\mathrm{in}} := \mathbf{D}_P : \mathbf{S} + (\mathbf{J}_0 \operatorname{Grad}\mathbf{D}_P) \circ \operatorname{Grad}\mathbf{S}, \tag{51}$$

where pairs of generalized velocities and forces (fluxes and affinities) are $\{\mathbf{D}_P,$ $\mathbf{J}_0 \operatorname{Grad}\mathbf{D}_P\}$ and $\{\mathbf{S}, \operatorname{Grad}\mathbf{S}\}$. It is very convenient to apply here Rice's normality

approach with PIR in the same way as for nonpolar case. Doing so, we obtain a new evolution equation for gradient of plastic stretching:

$$\frac{1}{\Lambda}\mathbf{J}_0 \operatorname{Grad}\mathbf{D}_P = \partial_{\operatorname{Grad}\boldsymbol{\sigma}}\Omega. \tag{52}$$

In order to illustrate applicability of this result, let us take a very simple extension of the previous nonpolar loading function (46) as follows:

$$2\,\Omega = (a_1 + a_3 s_{22})s_2 + a_2(s_1 s_2 - s_3). \tag{53}$$

This gives rise to new weakly nonlocal evolution equations

$$\mathbf{J}_0 \operatorname{Grad}\mathbf{D}_P = \Lambda\, a_3\, s_2 \operatorname{Grad}\mathbf{S}, \tag{54a}$$

$$\mathbf{D}_P = \Lambda\,(a_1 + a_2 s_1 + a_3 s_{22})\mathbf{S}_d/Y_0 - 3/2\,\Lambda\, a_2(\mathbf{S}_d^2)_d. \tag{54b}$$

The first of them does not exist in the nonpolar case, whereas the second is a modified evolution equation for plastic stretching which explicitly depends on the stress gradient through the invariant s_{22}. In both of these equations Λ is given by (47). We believe that a further exploitation of (52) with diverse distributions of monocrystal grains (and corresponding tesselations) within carefully selected diverse RVE could give us some new information about gradient viscoplasticity of polycrystals.

5. – Concluding remarks

The following general conclusions might be drawn from the above analysis:

– Geometrical analysis of polycrystalline thermo-inelastic micromorphic materials with approximately homogeneous grain strains is given. The simplest linear approximation is used for the homogenization applied. Corresponding balance laws as well as constitutive equations have been derived. A comparison with theories in [17, 16] reveals that the method proposed in this paper does not require any new material constants or scaling parameters. Nonpolar material constants suffice to build the theory, but detailed grain distribution and local symmetries must be known in advance.

– The thermodynamics applied here is based on Vakulenko's concept of thermodynamic time and tensor representation theory following [20]. For nonpolar case it was successfully compared with experimental results.

– New weakly nonlocal evolution equations for plastic stretching and its gradient have been derived. Their very simple version with only one additional material constant, with respect to nonpolar case, is shown explicitly.

We believe that further research in this area would be worthwhile. It would require explicit calculations for some prescribed grain forms within the RVE as well as diverse local material symmetries.

REFERENCES

[1] Mićunovic M., *Theor. Appl. Mech.*, **28-29** (2002) 235.
[2] Kröner E., *J. Eng. Mech. Div. Proc. ASCF* (1980) 106-889.
[3] Mićunović M., *Philos. Mag.* (2005) 4031.
[4] Kröner E., *Ration. Mech. Anal.*, **4** (1960) 273.
[5] Mićunović M., *Bull. Acad. Polon. Sci.-Ser. Sci. Techn.*, **22** (1974) 579, 633; **23** (1975) 89.
[6] Sidoroff F. and Teodosiu C., *Large Deformations of Solids: Physical Basis and Math. Modelling*, edited by Gittus J., Zarka J. and Nemat-Nasser S. (Elsevier, London) 1987.
[7] Stojanovic R., *Recent Development in the Theory of Polar Continua*, CISM Courses and Lectures **27** (Springer, Wien) 1972.
[8] Asaro R. J. and Lubarda V. A., *Mechanics of Solids and Materials* (Cambridge University Press, Cambridge) 2006.
[9] Zorawski M., private communication (1974).
[10] Mićunović M., *J. Mech. Behavior Mater.*, **4/4** (1993) 331.
[11] Maugin G. A., *The Thermomechanics of Plasticity and Fracture* (Cambridge University Press, Cambridge) 1992.
[12] Forest S., *Theor. Appl. Mech.*, **28-29** (2002) 113.
[13] Stojanovic R., *Phys. Status Solidi*, **2** (1962) 566.
[14] Teodosiu C., *Fund. Aspects Disl. Theory*, II, edited by Simmons J. A. *et al.*, Spec. Publ. **317** (Nat. Bur. Standards, Washington D.C.) 1970.
[15] Kröner E., *Statistical Continuum Mechanics*, CISM Course **92** (Springer, Wien) 1971.
[16] Lubarda V. A. and Markenscoff X., *J. Mech. Phys. Solids*, **48** (2000) 553.
[17] Fleck N. A. and Hutchinson J. W., *Adv. Appl. Mech.*, **33** (1997) 295.
[18] Maruszewski B. and Micunovic M., *Int. J. Eng. Sci.*, **27** (1989) 955.
[19] Spencer A. J. M., *Continuum Physics*, edited by Eringen A. C. (Academic Press, New York) 1971.
[20] Mićunović M., *Thermomechanics of Viscoplasticity: Fundamentals and Applications* (Springer, Berlin-Heidelberg) 2008.
[21] Fomin V., *Continuum Mechanics for Engineers* (Leningrad University Press, Leningrad) 1975 (in Russian).
[22] Vakulenko A. A., *Izv. Akad. Nauk SSSR, Mekh. Tverd. Tela*, **1** (1970) 69.
[23] Perzyna P., *Rev. Phys. Appl.*, **23** (1988) 445.
[24] Rice J. R., *J. Mech. Phys. Solids*, **19** (1971) 433.
[25] Mićunovic M., Albertini C. and Montagnani M., *Solid Mechanics*, edited by Hajdin N., Vol. **87/3** (Serbian Acad. Sci. Publ.) 1997.
[26] König J. A. and Olszak W., *Topics in Applied Continuum Mechanics*, edited by Zeman J. L. and Ziegler F. (Springer, Wien) 1974.