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Low order inelastic micromorphic polycrystals

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Abstract

The paper deals with some fundamental issues essential for constitutive modelling of plastic behaviour of metals. Geometric and kinematic aspects of intragranular as well as intergranular plastic deformation of polycrystals are discussed. Homogeneous grain strains are composed into the resulting behaviour of representative volume element (*RVE*). A homogenization of total, plastic and elastic strains has been done. Constitutive equations by a self consistent method have been discussed. A simplest case of higher gradient theory is discussed. Elastic strain is covered by the effective field homogenization method inside a RVE. It is underlined that plastic stretching and plastic spin are not independent.

1 Introduction

The principal objective of this work is to find a simplest yet realistic way of description of polycrystal behaviour of metals. In such a problem grains of diverse orientations meet at their boundaries where most dislocations are concentrated. Intergranular and intragranular plastic sliding must be accompanied by thermoelastic straining in order to preserve continuity of the body. Even without external forces residual stresses exist and due to discontinuous change of orientation of neighbouring

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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. Again the question arises to which part of strain to apply such an approach. The third issue which must analyzed is proper geometry of the considered thermo-inelastic strain history for such a polycrystalline body.

The exposition in this paper gives first geometrical analysis of finite thermo-inelastic strains of polycrystalline bodies. Here issue of micro and macro-rotations is especially considered. Then conditions for homogeneous total and/or elastic and plastic strains are formulated leading to balance laws. The same analysis has been applied to materials homogenized in such a way that deformation gradient, elastic and plastic distortion are linear functions of relative position inside RVE. Constitutive equations for stress and its moment are formulated by the effective field method. Finally, a brief account to evolution equations following mainly [18] is given. The interdependence between evolution equations for *plastic stretching* (often named by experimentalists as plastic strain rate tensor) and *plastic spin* is underlined.

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 scalar parameter allows for 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 [8, 13]). Of course, the corresponding *plastic distortion tensor*

$$\mathbf{F}_P(.,t) := \mathbf{F}_E(.,t)^{-1}\mathbf{F}(.,t), \tag{1}$$

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 above formula from the left hand side by $\mathbf{F}_E\ (.,t)$ we reach at original Kröner's decomposition rule which is often wrongly named as Lee's decomposition formula.

It is worthy of note that $curl\mathbf{F}_E\ (.,t)^{-1} \neq \mathbf{0}$ and this *incompatibility*(cf. [13]) is commonly connected to an asymmetric second order *tensor of dislocation density.*

For further considerations let us introduce vectors $d\mathbf{x} \in (k(t)), d\xi \in (n(t))$ and $d\mathbf{x}_0 \in (k(t_0))$ connecting two infinitesimally adjacent particles:

$$d\mathbf{x} = \mathbf{F}d\mathbf{x}_0,\ d\mathbf{x} = \mathbf{F}_E d\xi,\ d\xi = \mathbf{F}_P d\mathbf{x}_0. \tag{2}$$

2.1 Micro and macro rotations of RVE

In order to reduce an excessive use of indices and in accord with notation used in classical references like [25] 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. [25, 13])

$$\mathbf{F} = F^k_{.K}\mathbf{g}_k \otimes \mathbf{g}_0^K,\ \ \mathbf{\Phi} = \Phi^k_{.\lambda}\mathbf{g}_k \otimes \mathbf{h}^\lambda,\ \ \mathbf{\Pi} = \Pi^\lambda_{.K}\mathbf{h}_\lambda \otimes \mathbf{g}_0^K, \tag{3}$$

[1]Another more natural approach by [22] with $\mathbf{F}_P(.,t) := \mathbf{F}_E(.,t)^{-1}\mathbf{F}(.,t)\,\mathbf{F}_E(.,t_0)$ is less convienent for further analysis than the definition *(1)*. In fact, the formula *(1)*is slightly modified in [22] to account for the initial value of $\mathbf{F}_E(.,t)$ comparing $(n(t_0))$ and $(n(t))$ local configurations.

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.

Following [18] 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 to the considered slip plane (cf. [1]) 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

$$\mathbf{h}^\alpha_{\cdot\,\Lambda}(t) = \mathbf{R}_{\Lambda\Pi}(t)\, \mathbf{h}^\alpha(t), \tag{4}$$

where $\alpha \in \{1, 3\}$ and $\Lambda \in \{1, N\}$. 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 to

$$\mathbf{h}^\alpha(t) := \sum_\Lambda c_\Lambda \mathbf{h}^\alpha_{\cdot\,\Lambda}(t). \tag{5}$$

Clearly, the tensors $\mathbf{R}_{\Lambda\Pi}$, $(\Lambda \in \{1, N\})$ describe *relative plastic microrotations* of all grains with respect to average orientation of *RVE*. For monocrystal each of these vectors 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 $(n(t_0))$ we may write a formula analogous to (1) for the *micro-plastic distortion tensor*

$$\mathbf{\Pi}_\Lambda := \mathbf{\Pi}_{\Lambda E}\, \mathbf{\Pi}_{\Lambda P}, \tag{6}$$

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

$$\mathbf{s}_{\alpha\Lambda}(t) = S^\alpha_{\Lambda\beta}\mathbf{h}^\beta_{\cdot\,\Lambda}(t), \quad \mathbf{n}_{\alpha\Lambda}(t) = N^\alpha_{\Lambda\beta}\mathbf{h}^\beta_{\cdot\,\Lambda}(t), \tag{7}$$

where $S^{\alpha}_{\Lambda\beta} = const$ and $N^{\alpha}_{\Lambda\beta} = const$ we may write a representation for the micro-plastic distortion as follows:

$$\mathbf{\Pi}_{\Lambda P} = \mathbf{1} + \mathbf{R}_{\Lambda\Pi}(t) \left[\sum_{\alpha} \gamma_{\alpha\Lambda} S^{\alpha}_{\Lambda\beta} N^{\alpha}_{\Lambda\gamma} \mathbf{h}^{\beta}(t) \otimes \mathbf{h}^{\gamma}(t)) \right] \mathbf{R}^{T}_{\Lambda\Pi}(t) \tag{8}$$

On the other hand, assuming that residual micro-elastic rotation is negligibly small (cf. also [18]) [2] i.e. that by means of the polar decomposition $\mathbf{\Pi}_{\Lambda E} = \mathbf{U}^{res}_{\Lambda E} = \mathbf{V}^{res}_{\Lambda E}$ we may finally write

$$\mathbf{\Pi}_{\Lambda}(t) = \mathbf{V}^{res}_{\Lambda E}(t) \mathbf{R}_{\Lambda\Pi}(t) \left[\mathbf{1} + \sum_{\alpha} \gamma_{\alpha\Lambda} S^{\alpha}_{\Lambda\beta} N^{\alpha}_{\Lambda\gamma} \mathbf{h}^{\beta}(t) \otimes \mathbf{h}^{\gamma}(t)) \right] \mathbf{R}^{T}_{\Lambda\Pi}(t) \tag{9}$$

It is natural to connect macro (for *RVE*) and micro (for individual grains) plastic distortions by means of spatial averaging

$$\mathbf{\Pi}(t) = \langle \mathbf{\Pi}_{\Lambda}(t) \rangle \equiv \sum_{\Lambda} c_{\Lambda} \mathbf{\Pi}_{\Lambda}(t). \tag{10}$$

Let us apply the polar decomposition $\mathbf{\Pi} = \mathbf{R}_P \mathbf{U}_P$ to the macro plastic distortion introducing the macro-plastic rotation tensor $\mathbf{R}_P$ which is arbitrary (according to Zorawski [28]) and might be fixed either to be a unit tensor or to have the Mandel's isoclinicity property (cf. [15] 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 macro rotations are prepared. The two mentioned approaches are very useful to fix macro plastic rotations:*

1. *The first way of eliminating macro plastic rotation*

$$\mathbf{\Pi} = \mathbf{U}_P = \mathbf{C}_P^{1/2} \tag{11}$$

where $\mathbf{C}_P \equiv \mathbf{\Pi}^T \mathbf{\Pi}$ *greatly simplifies macro-plastic spin issue [15, 18].*

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

2. *The second way could be called Mandel's average macro isoclinicity by the identification:*

$$\mathbf{h}^{\alpha}(t) = \mathbf{h}^{\alpha}(t_0), \tag{12}$$

which approximately aligns plastically deformed RVE-elements 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 micro-plastic rotations must not be eliminated unless further tearing of RVE-elements is performed to size of monocrystal grains which is, by assumption, much smaller than typical dimension of RVE .

Joining *RVE*-elements in $(n(t))$ into a continuous body requires for each grain micro-elastic distortion $\mathbf{\Phi}_{\Lambda}$. Again polar decomposition allows: $\mathbf{\Phi}_{\Lambda} = \mathbf{R}_{\Lambda E}\mathbf{U}_{\Lambda E}$. Here the right micro-elastic stretch $\mathbf{U}_{\Lambda E}$ does not include the left micro-residual stretch $\mathbf{V}^{res}_{\Lambda E}$.

Recalling the Kröner's decomposition (1) we could make a new grouping of terms in the following way[3]

$$\mathbf{F}_{\Lambda} = \mathbf{R}_{\Lambda E}\ \mathbf{U}_{\Lambda E}\ \mathbf{V}^{res}_{\Lambda E}\ \mathbf{\Pi}_{\Lambda P} \equiv \mathbf{\Phi}_{\Lambda E}\ \mathbf{\Pi}_{\Lambda P} \tag{13}$$

Here $\mathbf{\Phi}_{\Lambda E}$ encompasses rotation of *RVE*-element 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 micro-plastic rotations.

2.2 Few notes on inelastic strains

If the micro-plastic deformation tensors for individual grains are (cf. (8))

$$\begin{aligned}\mathbf{C}_{\Lambda\Pi} \;=\; & \mathbf{\Pi}^T_{\Lambda P}\mathbf{\Pi}_{\Lambda P} \equiv \mathbf{1} + \mathbf{R}_{\Lambda\Pi}\left[\sum_{\alpha}\gamma_{\alpha\Lambda}\left(\mathbf{A}_{\alpha\Lambda} + \mathbf{A}^T_{\alpha\Lambda}\right)\right]\mathbf{R}^T_{\Lambda\Pi} \;+ \\ & \mathbf{R}_{\Lambda\Pi}\left[\sum_{\alpha}\gamma_{\alpha\Lambda}\mathbf{A}^T_{\alpha\Lambda}\right]\left[\sum_{\beta}\gamma_{\beta\Lambda}\mathbf{A}_{\beta\Lambda}\right]\mathbf{R}^T_{\Lambda\Pi}.\end{aligned} \tag{14}$$

[3]The following decomposition differs from the approach in [18] where micro-plastic distortion contains also micro-residual elastic strains.

then their volume average named *macro-plastic deformation tensor* $\mathbf{C}_P$ has the following form:

$$\mathbf{C}_P = \langle \mathbf{C}_{\Lambda\Pi} \rangle = \left\langle \mathbf{\Pi}_{\mathbf{\Lambda}}^{\mathbf{T}} \mathbf{\Pi}_{\Lambda} \right\rangle \equiv \sum_{\Lambda} c_{\Lambda} \mathbf{\Pi}_{\mathbf{\Lambda}}^{\mathbf{T}} \mathbf{\Pi}_{\Lambda} \neq \mathbf{\Pi}^{\mathbf{T}} \mathbf{\Pi} \tag{15}$$

and is different from product of averages of plastic distortions. This must be taken into account in all the subsequent derivations.

Suppose that we accept macro-isoclinicity assumption. Then taking $\mathbf{h}^{\alpha}(t) = \mathbf{h}^{\alpha}(t_0) = const$ and by making use of the relation $\dot{\mathbf{R}}_{\Lambda\Pi}\mathbf{R}_{\Lambda\Pi}^{T} = \mathbf{\Omega}_{\Lambda\Pi}$ for *relative plastic micro-spin* the relation (8) gives:

$$\begin{aligned} \dot{\mathbf{\Pi}}_{\Lambda P} &= \mathbf{R}_{\Lambda\Pi} \sum_{\alpha} \mathbf{A}_{\alpha\Lambda}\ \dot{\gamma}_{\alpha\Lambda} \mathbf{R}_{\Lambda\Pi}^{T} + \\ & \mathbf{\Omega}_{\Lambda\Pi} \left(\mathbf{\Pi}_{\Lambda P} - \mathbf{1} \right) + \left(\mathbf{\Pi}_{\Lambda P} - \mathbf{1} \right) \mathbf{\Omega}_{\Lambda\Pi}^{T}. \end{aligned} \tag{16}$$

Then velocity gradient at $\Lambda-$grain may be expressed by means of :

$$\mathbf{L}_{\Lambda} = \dot{\mathbf{\Phi}}_{\Lambda E}\ \mathbf{\Phi}_{\Lambda E}^{-1} + \mathbf{\Phi}_{\Lambda E} \dot{\mathbf{\Pi}}_{\Lambda P} \mathbf{\Pi}_{\Lambda P}^{-1} \mathbf{\Phi}_{\Lambda E}^{-1} \equiv \mathbf{L}_{\Lambda E} + \mathbf{\Phi}_{\Lambda E} \mathbf{L}_{\Lambda P} \mathbf{\Phi}_{\Lambda E}^{-1}. \tag{17}$$

such that the product $\mathbf{\Phi}_{\Lambda E}^{T} \mathbf{L}_{\Lambda} \mathbf{\Phi}_{\Lambda E}$ may be split into symmetric and antysymmetric parts as follows:

$$\mathbf{\Phi}_{\Lambda E}^{T} \mathbf{L}_{\Lambda} \mathbf{\Phi}_{\Lambda E} = \dot{\mathbf{E}}_{\Lambda E}\ + \mathcal{E}_{(n)} \omega_{\Lambda E} + \left(2\mathbf{E}_{\Lambda E} + \mathbf{1} \right) \mathbf{L}_{\Lambda P}, \tag{18}$$

where $\mathcal{E}_{(n)} = \mathcal{E}^{\alpha\beta\gamma} \mathbf{h}_{\alpha} \otimes \mathbf{h}_{\beta} \otimes \mathbf{h}_{\gamma}$ is Ricci tensor related to $(n\,(t)) -$ configuration, $\omega_{\Lambda E}$ is the elastic micro spin and $2\mathbf{E}_{\Lambda E} = \mathbf{\Phi}_{\Lambda E}^{T} \mathbf{\Phi}_{\Lambda E} - \mathbf{1}$ is the micro-elastic strain tensor.

On the other hand, if we accept eliminating macro plastic rotation, then obviously

$$2\ \mathbf{D}_P = \dot{\mathbf{U}}_P\ \mathbf{U}_P^{-1} + \mathbf{U}_P^{-1} \dot{\mathbf{U}}_P, \ \ 2\ \mathbf{W}_P = \dot{\mathbf{U}}_P\ \mathbf{U}_P^{-1} - \mathbf{U}_P^{-1} \dot{\mathbf{U}}_P, \tag{19}$$

i.e. macro-plastic stretching and spin are not independent. The above relations will be used in subsequent sections.

3 Balance laws

3.1 Low order polycrystals

Let us introduce a *mass distribution function* by means of

$$\varphi(\mathbf{x}') = \{\varphi_\Lambda(\mathbf{x}')|\mathbf{x}' \in \Delta V, \Lambda \in \{1, N\}\}, \tag{20}$$

with

$$\varphi_\Lambda(\mathbf{x}') = \{ \begin{array}{c} 1, \mathbf{x}' \in \Delta V_\Lambda \\ 0, otherwise. \end{array}$$

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

$$\int_{\Delta V} \varphi(\mathbf{x}')\mathbf{x}' dm' = \mathbf{x}\Delta m, \quad \int_{\Delta V_\Lambda} \varphi_\Lambda(\mathbf{x}'_0)\mathbf{x}^*_0 dm' = \mathbf{x}^*_{0\Lambda}\Delta m_\Lambda, \tag{21}$$

where 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 micro-strains.*

Such materials are called in this paper low order micromorphic polycrystals. Moreover, let center of a *RVE*-element 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:

$$\mathbf{F}' = \langle \mathbf{F}' \rangle + \mathbf{F}^* \equiv \mathbf{F} + \varphi_\Lambda(\mathbf{x}')\mathbf{F}^*_\Lambda, \quad (where\ \mathbf{x}' \in \Delta V_\Lambda)\,. \tag{22}$$

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

$$\mathbf{v}\Delta m = \int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}' dV' = \dot{\mathbf{x}}\Delta m, \tag{23}$$

$$\Delta \mathbf{l}_O = \int_{\Delta V} \varphi(\mathbf{x}')\mathbf{x}' \times \dot{\mathbf{x}}' dV' = \left(\mathbf{r} \times \mathbf{v} + \mathcal{E} : \sum_\Lambda c_\Lambda \mathbf{F}_\Lambda \mathbf{J}_{0\Lambda} \dot{\mathbf{F}}^T_\Lambda \right) \Delta m, \tag{24}$$

$$2\Delta T = \int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\dot{\mathbf{x}}' dV' = \left(\mathbf{v}\mathbf{v} + \sum_\Lambda c_\Lambda tr \left\{ \dot{\mathbf{F}}_\Lambda \mathbf{J}_{0\Lambda} \dot{\mathbf{F}}^T_\Lambda \right\} \right) \Delta m, \tag{25}$$

Here the *material grain micro-inertia tensor* (cf. also [25]) for a Λ-th grain equals to:

$$\mathbf{J}_{0\Lambda}\Delta m_{\Lambda} := \int_{\Delta V_{\Lambda}} \varphi_{\Lambda}(\mathbf{x}_0')\mathbf{x}_0^* \otimes \mathbf{x}_0^* dm'. \tag{26}$$

Remark 2 (Non-proportionality) *It is interesting to note here that due to symmetry properties of* $\mathbf{J}_{0\Lambda}$ *and antysymmetry of Ricci tensor* $\mathcal{E} = \mathcal{E}_{ijk}\mathbf{g}^i \otimes \mathbf{g}^j \otimes \mathbf{g}^k$ *the second term in (24) disappears for proportional strain paths whenever* $\mathbf{F}_{\Lambda}$ *and* $\dot{\mathbf{F}}_{\Lambda}$ *have same directions i.e. when* $\dot{\mathbf{F}}_{\Lambda} = \alpha\mathbf{F}_{\Lambda}, \alpha \in \Re$. *It should be noted that in general non-proportionality in strain histories affects very much experimental results for characterization of inelastic behaviour of metals (cf. e.g.. [16]).*

Consider now stresses and their moments in a *RVE*-element. 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

$$\mathbf{\Phi}' = \langle \mathbf{\Phi}' \rangle + \mathbf{\Phi}^* \equiv \mathbf{\Phi} + \varphi_{\Lambda}(\mathbf{x}')\mathbf{\Phi}_{\Lambda}^*, \quad \mathbf{\Pi}' = \langle \mathbf{\Pi}' \rangle + \mathbf{\Pi}^* \equiv \mathbf{\Pi} + \varphi_{\Lambda}(\mathbf{x}')\mathbf{\Pi}_{\Lambda}^* \tag{27}$$

also holds. At $\mathbf{x}' \in \Delta V_{\Lambda}$ let second Piola-Kirchhoff ($(n(t))$-related) and Cauchy stress be related by means of $\mathbf{\Phi}'\mathbf{S}'\mathbf{\Phi}'^T = \mathbf{T}'\, det\mathbf{\Phi}'$. Then Hooke's law at such a point has the form

$$\mathbf{S}' = \mathbb{D}' : \mathbf{E}_E' = \frac{1}{2}\varphi_{\Lambda}(\mathbf{x}')\mathbb{D}_{\Lambda} : \left(\mathbf{\Phi}_{\Lambda E}^T\mathbf{\Phi}_{\Lambda E}^T - \mathbf{1}_n\right) \equiv \varphi_{\Lambda}(\mathbf{x}')\mathbf{S}_{\Lambda} \tag{28}$$

and the macro-stress of *RVE* is obtained by the averaging[4]

$$\mathbf{S} = \langle \mathbf{S}' \rangle = \sum_{\Lambda} \mathbb{D}_{\Lambda} : \mathbf{E}_{\Lambda E}. \tag{29}$$

In our case of low order micromorphic polycrystals the forth rank tensor of elasticity has the form $\mathbb{D}_{\Lambda} = D^0_{\alpha\beta\gamma\delta}\, \mathbf{h}^{\alpha}_{\cdot\,\Lambda} \otimes \mathbf{h}^{\beta}_{\cdot\,\Lambda} \otimes \mathbf{h}^{\gamma}_{\cdot\,\Lambda} \otimes \mathbf{h}^{\delta}_{\cdot\,\Lambda}$ with $D^0_{\alpha\beta\gamma\delta} = const$. Let us introduce the notation $(\mathbb{R}_{\Lambda\Pi})_{\alpha\gamma\beta\delta} := (\mathbf{R}_{\Lambda\Pi} \diamond \mathbf{R}_{\Lambda\Pi})_{\alpha\gamma\beta\delta} \equiv$

[4]Even in the case of macro-homogeneous elastic distortion throughout the RVE due to different orientations of grain structures macro-elastic constants differ from their micro-elastic counterparts.

$(\mathbf{R}_{\Lambda\Pi})_{\alpha\beta}\,(\mathbf{R}_{\Lambda\Pi})_{\gamma\delta}$. With respect to average *RVE*-base in (n)-configuration we have the equivalent of (29) as follows:

$$\mathbf{S} = \sum_{\Lambda} \left(\mathbb{R}_{\Lambda\Pi} : \mathbb{D}^0 : \mathbb{R}^T_{\Lambda\Pi}\right) : \mathbf{E}_{\Lambda E}. \tag{30}$$

Remark 3 (Hill-Mandel) *In this and subsequent sections so-called Hill-Mandel principle of macrohomogeneity ([6, 12]) would be of great practical use allowing replacement of average of a product by the corresponding product of averages. To our regret there is not much justification for its application. Kröner calls it also ergodicity property in [6]. In statistical theories it is widely applied.*

The vector of stress moments for *RVE* is given by :

$$\begin{aligned}\Delta\mathbf{m}_O &= \int_{\partial\Delta V} \varphi(\mathbf{x}')\mathbf{x}' \times \mathbf{T}'\mathbf{n}' ds' = \int_{\Delta V} \varphi(\mathbf{x}') div\left(\mathbf{x}' \times \mathbf{T}'\right) dV' = \\ &\Delta V\left(\mathbf{x} \times div\mathbf{T} - \tau\right) + \sum_{\Lambda} \Delta S_{\Lambda}\left(\mathbf{x}^* \times [\![\mathbf{T}^*_{\Lambda}]\!]\ \mathbf{n}_{\Lambda}\right)|_{\partial\Delta V_{\Lambda}}\end{aligned} \tag{31}$$

Here again we have splitting $\mathbf{T}' = \langle\mathbf{T}'\rangle + \mathbf{T}^* = \mathbf{T} + \varphi_{\Lambda}(\mathbf{x}')\mathbf{T}^*_{\Lambda}$ for $\mathbf{x}' \in \Delta V_{\Lambda}$. and $\lceil\mathbf{T}^*_{\Lambda}\rceil$ denotes jump of the fluctuation of Cauchy stress on boundaries of Λ-th grain (cf. also [12]). The average Cauchy stress is here divided into its antysymmetric and symmetric parts by means of

$$\tau = \frac{1}{2}\mathcal{E}\colon \mathbf{T},\ \mathbf{T_a} = \mathcal{E}\tau \equiv \frac{\mathbf{1}}{\mathbf{2}}\left(\mathbf{T} - \mathbf{T^T}\right),\ \mathbf{T_s} = \frac{1}{2}\left(\mathbf{T} + \mathbf{T}^T\right) \equiv \sigma. \tag{32}$$

In the same way the mechanical working done by micro-stresses throughout *RVE* equals to:

$$\begin{aligned}\Delta P &= \int_{\partial\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\mathbf{T}'\mathbf{n}' ds' = \sum_{\Lambda} \Delta S_{\Lambda}\left(\mathbf{x}^* \times [\![\mathbf{T}^*_{\Lambda}]\!]\ \mathbf{n}_{\Lambda}\right)|_{\partial\Delta V_{\Lambda}} + \\ &\Delta V\left(\mathbf{T} : grad\dot{\mathbf{x}} + \dot{\mathbf{x}} div\mathbf{T} + \sum_{\Lambda} c_{\Lambda}\mathbf{T}^*_{\Lambda} : grad\dot{\mathbf{x}}^*_{\Lambda}\right).\end{aligned} \tag{33}$$

Now we are ready to write balance equations for typical *RVE.* First, balance of momentum leads to the traditional non-polar equation by means of:

$$\frac{D}{Dt}\int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}' dV' = \int_{\partial\Delta V} \varphi(\mathbf{x}')\mathbf{T}'\mathbf{n}' ds' \quad \Rightarrow \quad \rho\ddot{\mathbf{x}} = div\mathbf{T}, \tag{34}$$

whereas balance of moment of momentum $D\Delta\mathbf{l}_O/Dt = \Delta\mathbf{m}_O$ gives the antysymmetric part of Cauchy stress as follows:

$$2\tau = -\rho\mathcal{E}\colon \sum_{\Lambda} c_\Lambda \mathbf{F}_\Lambda \mathbf{J}_\Lambda \ddot{\mathbf{F}}_\Lambda^T + \frac{1}{\Delta V}\sum_{\Lambda}\ \Delta S_\Lambda \left(\mathbf{x}^* \times [\![\mathbf{T}_\Lambda^*]\!]\ \mathbf{n}_\Lambda\right)|_{\partial\Delta V_\Lambda}\ . \quad (35)$$

Looking at the above formula we may draw the conclusion that for low order micromorphic polycrystals stress is symmetric only if the two following conditions are satisfied:

Condition 1 (Intergranular continuity) *stress vector is continuous on grain boundaries and*

Condition 2 (Proportional paths) *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.

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

$$\Delta\dot{T} + \Delta\dot{E} = \Delta P + \Delta Q, \quad (36)$$

where $\Delta\dot{E}$ is time rate of internal energy, while ΔP and ΔQ are mechanical and non-mechanical working which includes thermal effects. If the average velocity gradient tensor $\mathbf{L} \equiv grad\dot{\mathbf{x}}$ is split into its symmetric and antysymmetric parts:

$$\omega = \frac{1}{2}\mathcal{E}\colon \mathbf{L},\ \mathbf{L_a} = \mathcal{E}\omega \equiv \frac{1}{2}\left(\mathbf{L} - \mathbf{L^T}\right),\ \mathbf{D} = \frac{1}{2}\left(\mathbf{L} + \mathbf{L}^T\right) \equiv \mathbf{L_s}, \quad (37)$$

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

$$2\tau\omega + \sum_{\Lambda} c_\Lambda \left(\sigma_\Lambda^*\colon \mathbf{D}_\mathbf{\Lambda}^* + 2\tau_\Lambda^*\omega_\Lambda^*\right) + \frac{1}{\Delta V}\sum_{\Lambda}\ \Delta S_\Lambda \left(\dot{\mathbf{x}}^* [\![\mathbf{T}_\Lambda^*]\!]\ \mathbf{n}_\Lambda\right)|_{\partial\Delta V_\Lambda} -$$
$$\frac{1}{2}\rho\sum_{\Lambda} c_\Lambda tr\left\{\ddot{\mathbf{F}}_\Lambda \mathbf{J}_\Lambda \dot{\mathbf{F}}_\Lambda^T + \dot{\mathbf{F}}_\Lambda \mathbf{J}_\Lambda \ddot{\mathbf{F}}_\Lambda^T\right\} = \rho\ \dot{e} - \sigma : \mathbf{D}. \quad (38)$$

3.2 A comment on homogenization

Let us describe now approximately grain behaviour by some smooth functions. 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.

$$\bar{\mathbf{F}}'=\bar{\mathbf{F}}+\mathcal{F}\mathbf{x}_0^*,\ \ \bar{\mathbf{\Phi}}'=\bar{\mathbf{\Phi}}+\mathbf{x}^*\mathcal{F}_E,\ \ \bar{\mathbf{\Pi}}'=\bar{\mathbf{\Pi}}+\mathcal{F}_P\mathbf{x}_0^*. \tag{39}$$

Now, the approximating "constants" $\bar{\mathbf{F}}$ and $\mathcal{F}$ are found by minimization of the functional

$$I=\frac{1}{\Delta V}\int_{\Delta V}\left\|\bar{\mathbf{F}}'-\mathbf{F}'\right\|^2 dV'\ . \tag{40}$$

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

$$\min_{(\bar{\mathbf{F}},\mathcal{F})} I \Rightarrow \left(\bar{\mathbf{F}},\mathcal{F}\right).$$

Taking the inner product as a means to form the above norm we get:

$$\bar{\mathbf{F}}=\mathbf{F}\quad\text{as well as}\quad \mathcal{F}=\left\langle\mathbf{F}^*\otimes\mathbf{x}_0^*\right\rangle\left\langle\mathbf{J}_0\right\rangle^{-1}. \tag{41}$$

In the same way we obtain approximating "constants" for the distortions: [5]

$$\bar{\mathbf{\Pi}}=\mathbf{\Pi}\quad\text{as well as}\quad \mathcal{F}_P=\left\langle\mathbf{\Pi}^*\otimes\mathbf{x}_0^*\right\rangle\left\langle\mathbf{J}_0\right\rangle^{-1}. \tag{42}$$

$$\bar{\mathbf{\Phi}}=\mathbf{\Phi}\quad\text{as well as}\quad \mathcal{F}_E=\left\langle\mathbf{J}\right\rangle^{-1}\left\langle\mathbf{x}^*\otimes\mathbf{\Phi}^*\right\rangle, \tag{43}$$

where the *spatial grain micro-inertia tensor* has the following form:

$$\mathbf{J}_\Lambda\Delta m_\Lambda:=\int_{\Delta V_\Lambda}\varphi_\Lambda(\mathbf{x}')\mathbf{x}^*\otimes\mathbf{x}^*dm'. \tag{44}$$

Remark 4 (Dislocation densities) *Antysymmetric parts of $\mathcal{F}_E$ and $\mathcal{F}_P$ are third order true spatial and material dislocation density tensors (cf. [24, 26, 13]):*

$$\mathbf{A}_E=\mathcal{E}:\mathcal{F}_E,\ \ \mathbf{A}_P=\mathcal{F}_P:\mathcal{E}_0. \tag{45}$$

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

where Ricci permutation tensor in material coordinates $\mathcal{E}_0 = \mathcal{E}_{KLM}\mathbf{g}_0^K \otimes \mathbf{g}_0^L \otimes \mathbf{g}_0^M$ *is used in the second relationship. The two representations 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.. [13]) but have to be omitted for the sake of brevity.

For further analysis of constitutive equations we will need balance laws for such a smoothed *RVE*. On the other hand the moment of momentum becomes (with a synonymous $D\mathcal{F}/Dt \equiv \mathcal{F}_t$):

$$\frac{\Delta \mathbf{l}_O}{\Delta m} = \frac{1}{\Delta m}\int_{\Delta V} \varphi(\mathbf{x}')\mathbf{x}' \times \dot{\mathbf{x}}' dV' = \mathbf{r} \times \mathbf{v} \; + \tag{46}$$
$$\mathcal{E} : \left(\mathbf{F}\mathbf{J}_0\dot{\mathbf{F}}^T + \mathbf{F}\mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F} : \mathcal{J}_0\dot{\mathbf{F}}^T + \mathcal{F} : \mathbb{J}_0 : \mathcal{F}_t^T\right),$$

where higher order inertia moments are given by (cf. also [6]):

$$\mathcal{J}_0 := \int_{\Delta V} \varphi(\mathbf{x}_0')\, \mathbf{x}_0^* \otimes \mathbf{x}_0^* \otimes \mathbf{x}_0^*\, dm', \quad \mathbb{J}_0 := \int_{\Delta V} \varphi(\mathbf{x}_0')\, \mathbf{x}_0^* \otimes \mathbf{x}_0^* \otimes \mathbf{x}_0^* \otimes \mathbf{x}_0^*\, dm'.$$

The balance equation for momentum has the same form as (34) while the balance equation of moment of momentum with the above linear approximation becomes:

$$2\tau\ \Delta V - \sum_{\mathbf{\Lambda}} \int_{\partial \mathbf{\Delta V_\Lambda}} (\mathbf{x}^* \times [\![\mathbf{T}_{\mathbf{\Lambda}}^*]\!]\ \mathbf{n}_{\mathbf{\Lambda}})\ dS'_\Lambda = -\rho\mathcal{E}\colon \Big(\mathbf{F}\mathbf{J}_0\ddot{\mathbf{F}}^T +$$
$$\mathcal{F} : \mathbb{J}_0 : \mathcal{F}_{tt}^T\Big) - \rho\mathcal{E} : \frac{D}{Dt}\left(\mathbf{F}\mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F} : \mathcal{J}_0\dot{\mathbf{F}}^T\right). \tag{47}$$

The expression for kinetic energy of *RVE* is obtained in the same way:

$$2\frac{\Delta T}{\Delta m} = \frac{1}{\Delta m}\int_{\Delta V} \varphi(\mathbf{x}')\dot{\mathbf{x}}'\dot{\mathbf{x}}' dV' = \mathbf{v}\mathbf{v} \; + tr\left(\dot{\mathbf{F}}\mathbf{J}_0\dot{\mathbf{F}}^T\right) +$$
$$tr\left(\dot{\mathbf{F}}\mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F}_t : \mathcal{J}_0\dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}_t^T\right). \tag{48}$$

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

$$\mathbf{D}' = \mathbf{D} + \mathbf{x}^* grad\mathbf{D}, \quad \omega' = \omega + \mathbf{x}^* grad\omega, \tag{49}$$

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

$$\begin{aligned} \frac{\Delta P}{\Delta V} - \dot{\mathbf{x}}\, div\mathbf{T} - \sigma : \mathbf{D} \ &= \ 2\tau\omega + \mathcal{M} \circ grad\mathbf{D} + 2\mathbf{M} : grad\omega + \\ &\frac{1}{\Delta V}\sum_{\mathbf{\Lambda}} \int_{\partial \mathbf{\Delta V_\Lambda}} (\dot{\mathbf{x}} \ [\![\mathbf{T}^*_{\mathbf{\Lambda}}]\!] \ \mathbf{n_\Lambda})\, dS'_\Lambda, \end{aligned} \tag{50}$$

where moments of the symmetric and antysymmetric stress are respectively:

$$\mathcal{M}\ \Delta V = \int_{\Delta V} \sigma^* \otimes \mathbf{x}^*\ dV', \quad \mathbf{M}\ \Delta V = \int^*_{\Delta V} \tau^* \otimes \mathbf{x}^*\ dV', \tag{51}$$

and vanish for homogeneous stress inside *RVE*-element. Finally, by means of relations (48) and (50) energy conservation equation (36) for *RVE* obtains the following form (by $\mathbf{q}$ the average heat flux vector is denoted i.e. $\mathbf{q} = \langle \mathbf{q}' \rangle$):

$$\begin{aligned} &\rho\ \dot{e} - \sigma : \mathbf{D} - div\mathbf{q} = \\ &\rho \tfrac{D}{Dt} tr\left(\dot{\mathbf{F}}\mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F}_t : \mathcal{J}_0\dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}_t^T\right) + \\ &2\tau\omega + \mathcal{M} \circ grad\mathbf{D} + 2\mathbf{M} : grad\omega + \rho \tfrac{D}{Dt}\ tr\left\{\dot{\mathbf{F}}\mathbf{J}_0\dot{\mathbf{F}}^T\right\} + \\ &\tfrac{1}{\Delta V}\textstyle\sum_{\mathbf{\Lambda}} \int_{\partial \mathbf{\Delta V_\Lambda}} (\dot{\mathbf{x}} \ [\![\mathbf{T}^*]\!] \ \mathbf{n})\, dS'_\Lambda. \end{aligned} \tag{52}$$

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 (52) 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 σ'_S and τ'_S, while elastic stretching is nothing but $\dot{\mathbf{E}}'_E$ and antysymmetric part of elastic "velocity gradient", denoted by $\mathbf{L}'_E := \dot{\mathbf{\Phi}}' \left(\mathbf{\Phi}'\right)^{-1}$, is given by the vector ω'_E. Then the energy conservation equation may be transformed into:

$$\begin{aligned} \rho_0\, \dot{e} - Div\mathbf{q}_{(n)} \;=\; & \rho_0 \frac{D}{Dt} tr\left(\dot{\mathbf{F}}\mathcal{J}_0 : \mathcal{F}_t^T + \mathcal{F}_t : \mathcal{J}_0\dot{\mathbf{F}}^T + \mathcal{F}_t : \mathbb{J}_0 : \mathcal{F}_t^T\right) + \\ & \sigma_S : \dot{\mathbf{E}}_E + \mathcal{M}_S \circ Grad\dot{\mathbf{E}}_E + \\ & 2\tau_S\omega_E + 2\mathbf{M}_S : Grad\omega_E + \\ & \rho_0 \frac{D}{Dt}\, tr\left\{\dot{\mathbf{F}}\mathbf{J}_0\dot{\mathbf{F}}^T\right\} + R\left(\dot{\mathbf{\Pi}}, Grad\dot{\mathbf{\Pi}}\right), \end{aligned} \tag{53}$$

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

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

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

$$\mathcal{M}_S\, \Delta V_0 = \int_{\Delta V} \sigma_S^* \otimes \xi^*\, dV'_0, \quad \mathbf{M}_S\, \Delta V_0 = \int_{\Delta V}^{*} \tau_S^* \otimes \xi^*\, dV'_0. \tag{54}$$

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 start with Hooke's law for each grain and compose them into RVE. For an arbitrary point inside *RVE* we obtain by means of (28) the following expression:

$$2e' = \mathbf{E}'_E : \mathbb{D}' : \mathbf{E}'_E = \left(\mathbf{E}_E + \mathbf{E}^*_E\right) : \left(\mathbb{D} + \mathbb{D}^*\right) : \left(\mathbf{E}_E + \mathbf{E}^*_E\right). \tag{55}$$

where again $\mathbb{D}' = \mathbb{R}'_\Pi : \mathbb{D}_0 : \mathbb{R}'^T_\Pi = \varphi_\Lambda(\mathbf{x}')\mathbb{D}_\Lambda$ depends on grain orientations. Averaging the above relation ship leads to:

$$
\begin{aligned}
2e &= 2e_{HM} + \left(\mathbf{J}_{(n)} Grad\mathbf{E}_E : \mathbb{D}_0^T\right) \circ Grad\mathbf{E}_E + \\
&\quad \mathbf{E}_E : \langle \mathbb{D}^* \otimes \xi^* \rangle \circ \left(Grad\mathbf{E}_E\right)^T + \\
&\quad Grad\mathbf{E}_E \circ \langle \xi^* \otimes \mathbb{D}^* \rangle : \mathbf{E}_E + \\
&\quad Grad\mathbf{E}_E \circ \langle \xi^* \otimes \mathbb{D}^* \otimes \xi^* \rangle \circ \left(Grad\mathbf{E}_E\right)^T
\end{aligned} \tag{56}
$$

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

Suppose that inertial higher order terms in () are negligible. Now, our averaged internal energy function contains only elastic strain and its gradient. Its differentiation and replacement into (53) leads to constitutive restrictions for symmetric part of stress tensor and its moment as follows:

$$
\begin{aligned}
\tfrac{1}{\rho_0}\sigma_S &= \tfrac{\partial e}{\partial \mathbf{E}_E} = \\
&\quad \mathbb{D}_0 : \mathbf{E}_E + \langle \mathbb{D}^* \otimes \xi^* \rangle \circ \left(Grad\mathbf{E}_E\right)^T,
\end{aligned} \tag{57}
$$

$$
\begin{aligned}
\tfrac{1}{\rho_0}\mathcal{M}_S &= \tfrac{\partial e}{\partial Grad\mathbf{E}_E} = \\
&\quad \mathbf{J}_{(n)} Grad\mathbf{E}_E : \mathbb{D}_0^T + \langle \xi^* \otimes \mathbb{D}^* \rangle : \mathbf{E}_E + \\
&\quad \langle \xi^* \otimes \mathbb{D}^* \otimes \xi^* \rangle \circ \left(Grad\mathbf{E}_E\right)^T.
\end{aligned} \tag{58}
$$

As already remarked antysymmetric stress and its gradient are negligible if higher order inertial terms can be disregarded. Two special cases of the above constitutive relations are of special interest to us.

Remark 5 (Isotropic grains) *Suppose that each grain is elastically isotropic which means* $\mathbb{D}' = \mathbb{D}_0(\lambda, \mu)$, *or, equivalently,* $\mathbb{D}^* = 0$. *Then*

$$
\begin{aligned}
2e &= \lambda \left(tr\mathbf{E}_E\right)^2 + 2\mu\ tr\left(\mathbf{E}_E^2\right) \mathbf{J}_{(n)} + \\
&\quad \lambda \mathbf{J}_{(n)} : \left[Grad\left(tr\mathbf{E}_E\right) \otimes Grad\left(tr\mathbf{E}_E\right)\right] + \\
&\quad 2\mu \left(\mathbf{J}_{(n)} Grad\mathbf{E}_E\right) \circ Grad\mathbf{E}_E.
\end{aligned}
$$

The main advantage of this expression is that it does not need any new material constant. The micro-inertia 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. [11] formula (42)) they have one additional constant and an unknown scaling length. As another example, Fleck and Hutchinson in [3] have five additional material constants and apply so-called* J_2*-theory in discussing their influence on overall inelastic behaviour of RVE.*

Remark 6 (Small grain rotations) *The second case of interest is slight disorder in Kröner's terminology (cf. [7]). In order words unlike Kröner's perfect disorder here relative grain rotations* $\mathbf{R}' = \mathbf{1} + \mathbf{R}^*$ *are so small that higher order products of* $\mathbf{R}^*$ *in* $\mathbb{D}'$ *may be neglected. Then* $D'^{\alpha\beta\gamma\delta} = D_0^{\alpha\beta\gamma\delta} + R^{*\alpha}_{\cdot\kappa}\ D_0^{\kappa\beta\gamma\delta} + R^{*\beta}_{\cdot\kappa}\ D_0^{\alpha\kappa\gamma\delta} + R^{*\gamma}_{\cdot\kappa}\ D_0^{\alpha\beta\kappa\delta} + R^{*\delta}_{\cdot\kappa}\ D_0^{\alpha\beta\gamma\kappa}$. *In this case an approximate symmetry of the whole RVE may be established around average structural vectors. Of special interest would be here to make inquiry about so-called defective invariants with respect to such average directions.*

4.2 Hooke's law by self-consistent method

In the paper [18] *effective field approach* was applied in deriving constitutive equation for stress related to $(n\,(t))$. In homogenization theories for composites with particulate inclusions this approach is based on assumption that each inclusion (in our case grain) behaves approximately as isolated and situated into the matrix with elasticity constants $\mathbb{D}_M$ while influence of neighboring inclusions is taken into account by means of the effective field $\mathbf{E}_{eff}$ acting on the considered inclusion [9].

Applying previous geometric considerations we may write Hooke's law for the $\Lambda-$grain in the form $\mathbf{S}_\Lambda = \mathbb{D}_\Lambda : \mathbf{E}_{\Lambda E}$. Then its volume averaging throughout the RVE gives the familiar equation of homogenization approach

$$\langle \mathbf{S}_\Lambda \rangle = \mathbb{D}_\Lambda : \langle \mathbf{E}_{\Lambda E} \rangle\,, \quad i.e.\ \ \mathbf{S} = \mathbb{D}_{eff} : \mathbf{E}_E. \tag{59}$$

In the paper [10] the author proposed the approach that for polycrystals the considered grain is understood as an inclusion in the matrix composed by all the other grains applying in this way the effective field approach. If instead of an infinite medium we employ this reasoning to the considered RVE then a direct application of the Levin's expression for the effective elastic moduli fourth rank tensor may be written as follows (index "M" stands for matrix while the notation $\langle\bullet\rangle_{\omega}$ means averaging by orientation only):

$$\mathbb{D}_{eff} = \mathbb{D}_M + [\mathbb{D}]\ (\mathbb{I} - \langle\mathbb{A}\mathbb{P}\rangle_{\omega}\ [\mathbb{D}]\ )^{-1} \langle\mathbb{A}\rangle_{\omega}\,,\ \ where\ \ \mathbb{D}_M \equiv \langle\mathbb{D}\rangle_{\omega}\,. \quad (60)$$

Here $(\mathbb{I})_{abcd} = \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}$ is the unit fourth rank tensor and

$$\mathbb{P}_{\Lambda}{=}\mathbb{S}_{\Lambda}^{-1}\mathbb{D}_M \equiv -\int_{\Delta V_{\Lambda}} \mathbb{K}(x-x')\ dV',\ \ with\ \ (\mathbb{K})_{abcd} = (\partial_a\partial_d G_{ac})_{(ab)}\,,$$

$$\mathbb{A}_{\Lambda} = (\mathbb{I} + \mathbb{P}_{\Delta}\ [\mathbb{D}]\ )^{-1},\ \ with\ \ [\mathbb{D}] = \mathbb{D}_{\Lambda} - \mathbb{D}_M.$$

In the above $\mathbb{S}_{\Lambda}$ is the Eshelby's tensor and $\mathbf{G}$ is the Green's function for the considered anisotropic crystal. The above expressions mean in fact application of Levin's formulae to our geometrical scheme. They may be used for an analytical determination of the effective elastic constants. What is really needed here is their extension to strain gradient case and comparison with formulae derived in previous section.

4.3 Evolution equation

According to the principle of inelastic memory introduced in [15] the second Piola-Kirchhoff stress is given by a very general functional accounting for plastic strain as well as plastic strain rate history as follows:

$$\mathbf{S}(t) = \mathcal{F}_{\tau=0}^{\infty}\,[\varepsilon_P(t-\tau), \dot{\varepsilon}_P(t-\tau)], \quad (61)$$

where the macro-plastic strain tensor could be for instance $\varepsilon_P = \mathbf{U}_P - \mathbf{1}$. When this functional may be represented by a nonlinear function of plastic strain and plastic strain rate the plastic material is of *differential type* (cf. [15]). Solving such an equation in plastic strain rate we would obtain the following evolution equation

$$\dot{\varepsilon}_P = \dot{\varepsilon}_P\,(\mathbf{S},\varepsilon_P) \quad (62)$$

in its standard form. By means of tensor representation theory [23, 15] it can be explicitly written as follows (MacAuley bracket $< f >= 1$ if plastic deformation takes place and $< f >= 0$ inside each elastic range):

$$\begin{aligned}\dot{\mathbf{U}}_P &= < f > [\, d_1(\chi)\mathbf{1} + d_2(\chi)\mathbf{U}_P + d_3(\chi)\mathbf{U}_P^2 + \\ &\quad d_4(\chi)\mathbf{S} + d_5(\chi)\mathbf{S}^2 + d_6(\chi)(\mathbf{S}\mathbf{U}_P + \mathbf{U}_P\mathbf{S}) + \\ &\quad d_7(\chi)(\mathbf{S}^2\mathbf{U}_P + \mathbf{U}_P\mathbf{S}^2) + d_8(\chi)(\mathbf{S}\mathbf{U}_P^2 + \mathbf{U}_P^2\mathbf{S})\,].\end{aligned} \tag{63}$$

Let us apply in the sequel the assumption of absence of macro-plastic rotations. Then from (19) immediately follows interconnexion between macro-plastic stretching and macro-plastic spin. Such a conclusion may be derived for average macro-isoclinicity (cf.[15] for details) but the procedure is much more tedious..

Remark 7 (Experiments) *In the paper [16] the authors derived from experimental evidence the following very simple evolution equation for macro-plastic stretching tensor*

$$\mathbf{D}_P = \dot{\sigma}_{eq}\, J(0)\, \pi^{\beta}\ \left[c_1\mathbf{S}_d + c_2(\mathbf{S}_d^2)_d\right] \tag{64}$$

under the assumption that the loading function type normality derived by Rice in [20] holds i.e. that $\mathbf{D}_P = \Lambda\, \partial_{\mathbf{S}}\Omega$ *holds. It should be mentioned that the equation is a special case of (63).*

In the above formulae $\dot{\pi} = \|\mathbf{D}_P\|$ *is the so called equivalent plastic strain rate,* $\mathbf{S}_d$ *is the deviatoric part of the Piola-Kirchhoff stress* $\mathbf{S}$, $\sigma_{eq} \equiv \|\mathbf{S}_d\|$ *denotes the equivalent Mises stress, whereas the integral kernel* J *of the integral equation*

$$\pi(t) = \int_0^t J(t-t')\ \dot{\sigma}_{eq}(t')\ dt' \tag{65}$$

is dependent on the initial equivalent stress rate as follows:

$$J(t-t') = \begin{cases} 0, & t' \geq t^*, \\ \exp(-M), & t' < t^*. \end{cases} \tag{66}$$

Here it is assumed that plastic straining initiates at a time t^* *when the equivalent stress reaches the critical stress rate dependent initial yield*

stress $Y_0\left(\dot{\sigma}_{eq}\right)$, *such that* $\sigma_{eq}(t^*) = Y_0\left[\dot{\sigma}_{eq}(t^*)\right]$. *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. A special attention deserves the assumed normality (64) and a detailed discussion on it as well as on non-locality is given in [18] criticizing the normality assumption. Anyway, the very simple equation (64) with just three material constants namely,* c_1, c_2, β *and one universal constant* M *[16] showed high agreement with multiaxial experiments from very low* ($D\pi \sim 0.001\ s^{-1}$) *to very high strain rates* ($D\pi \sim 1000\ s^{-1}$).

Let the specific free energy of the considered body be of the form

$$f = f_E\left(\mathbf{E}_E, T\right) + f_P\left(\lambda, T\right) \tag{67}$$

where λ is the isotropic hardening parameter given by

$$\begin{aligned} \dot{\lambda} \;:=\; & \mathbf{T} : \mathbf{D} - \mathbf{S} : \dot{\mathbf{E}}_E = \\ & \frac{1}{2}\mathbf{S} : \left(\mathbf{C}_E \dot{\mathbf{U}}_P \mathbf{U}_P^{-1} + \mathbf{C}_E \mathbf{U}_P^{-1} \dot{\mathbf{U}}_P\right) \equiv \mathbf{S}_U \colon \dot{\mathbf{U}}_P, \end{aligned} \tag{68}$$

having the meaning of plastic power. By means of the dissipation appearing in the second law of thermodynamics, namely $\vartheta \equiv \rho\,\dot{s} + div(\mathbf{q}/T) \geq 0$ Since the free energy is assumed in the form (67) we have $T\vartheta = \left(1 - \rho\partial_\lambda f\right)\dot{\lambda}$. By making use of this dissipation Vakulenko introduced a concept of *thermodynamic time* [27] by the following hereditary function

$$\zeta(t) := \int_0^t \psi[T\vartheta(t')]\, dt' \tag{69}$$

where T is the absolute temperature and s - the specific entropy. 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 (for instance, $\varepsilon_P = \mathbf{U}_P - \mathbf{1}$) is a functional of stress and stress rate history such that:

$$\varepsilon_P(\zeta) = \int_0^\zeta \mathbf{\Phi}\left[\zeta - \xi, \mathbf{S}(\xi), \dot{\mathbf{S}}(\xi), \pi(\xi)\right] d\xi. \tag{70}$$

In [18] the accumulated plastic strain $\pi(\zeta) \equiv \int_0^\zeta \|\dot{\varepsilon}_P(\xi)\|\, d\xi$ is added extending in such a way Vakulenko's arguments. Of course, this integral equation is adopted to our case of finite macro-plastic strains and absence of macro-plastic rotation. Differentiation of (70) with respect to the thermodynamic time gives:

$$\begin{aligned} \partial_\zeta \varepsilon_P &= \mathbf{\Phi}\left[0, \mathbf{S}(\zeta), \dot{\mathbf{S}}(\zeta), \pi(\zeta)\right] + \\ &\int_0^\zeta \partial_\zeta \mathbf{\Phi}\left[\zeta - \xi, \mathbf{S}(\xi), \dot{\mathbf{S}}(\xi), \pi(\xi)\right]\, d\xi. \end{aligned} \tag{71}$$

When the tensorial kernel in (70) is chosen in such a way that

$$\begin{aligned} &\mathbf{\Phi}\left[\zeta - \xi, \mathbf{S}(\xi), \dot{\mathbf{S}}(\xi), \pi(\xi)\right] = \\ &J(\zeta - \xi)\ \partial_\xi \sigma_{eq}(\xi) \mathbf{\Phi}_1\left(\mathbf{S}(\xi), \pi(\xi)\right) + \mathbf{\Phi}_2\left(\mathbf{S}(\xi), \pi(\xi)\right) \end{aligned} \tag{72}$$

and $\partial_\zeta J(\zeta - \xi) = 0$ (cf. (66)), then the integral on the right hand side of (70) vanishes. If, moreover the function in (69) is of the power type i.e. $\psi[T\vartheta] = (T\vartheta)^a$, then a multiplication of (71) by $\dot{\zeta}$ transforms this equation into

$$\dot{\mathbf{U}}_P = \mathbf{\Phi}_1 J(0)\, \dot{\sigma}_{eq} + \mathbf{\Phi}_2 \dot{\zeta}. \tag{73}$$

Its multiplication by $\mathbf{S}_U$ allows further $\dot{\lambda} = i_1 J(0)\, \dot{\sigma}_{eq} + i_2 \left(1 - \rho \partial_\lambda f\right)^a \dot{\lambda}^a$ where $i_\alpha = \mathbf{S}_U \colon \mathbf{\Phi}_\alpha,\ \alpha \in \{1, 2\}$. The explicit solution of this equation i.e. $\dot{\lambda} = \dot{\lambda}(\dot{\sigma}_{eq}, i_1, i_2)$ depends on the value of the exponent a. If value $a = 1$ suggested in [27] is taken, then the correction introduced by means of the tensor $\mathbf{\Phi}_2$ seems unnecessary apart from the stress rate dependent kernel $J(\zeta - \xi)$ (cf. (66)). However, taking a different from Vakulenko's value i.e. $a \neq 1$ the difference becomes significant. For example $a < 1$ may be named *decelarated ageing* whereas $a > 1$ would define *accelarated ageing.* By such a classification the value $a = 1$ might be termed as *steady ageing.* Nonsteady ageing is analyzed in detail in [18] with special account of values $a = 1/2$ and $a = 2$. According to [18] the case of steady ageing is not able to describe stress dependent creep process.

If $\mathbf{\Phi}_2$ is negligibly small, then evolution equation (71) obtains the form of (64). Accordingly, the evolution equation (64) belongs to the class of hereditary equations with thermodynamic time introduced by Vakulenko.

5 Concluding remarks

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

A) Geometrical analysis of thermo-inelastic polycrystal strains has been given.

B) Balance laws as well as constitutive equations with minimal number of material constants have been derived with special account on confrontation of homogeneous grain strains and a linear smoothing homogenization results.

C) Although successfully compared with experimental results evolution equations based on Vakulenko's concept of thermodynamic time and tensor representation theory have to be connected to inelastic slip micromechanisms following the same approach as for constitutive equations for stress and moment stress.

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Neelastični mikromorfni polikristali niskog reda

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Posmatraju se neke osnovne postavke esencijalne za konstitutivno modeliranje plastičnog ponašanja metala. Geometrijski i kinematski aspekti intragranularne kao i intergranularne plastične deformacije polikristala su diskutovane. Pritom su homogene deformacije zrna komponovane u rezultujuće ponašanje *reprezentativnog zapreminskog elementa* (*RVE*). Izvedena je homogenizacija totalne, plastične i elastične deformacije. Diskusija konstitutivnih jednačina je izvršena samousaglašavajućim metodom. Najprostiji slučaj teorije viših gradijenata je prikazan. Elastična deformacija je propisana homogenizacionim meto-dom efektivnog polja unutar RVE. Naglašeno je da brzina plastične deformacije i plastični spin nisumedjusobno nezavisni.