# Macro-modelling of thermo-inelastic composites

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THIS PAPER proposes a formulation of thermomechanics in which the thermodynamical processes can be subjected to the known a priori global constraints. On this basis the local (macro-constructive) and global (related to the whole composite body) averaged computational models of certain thermo-inelastic composites are derived.

W pracy przedstawiono podejście do termodynamiki, w którym procesy termodynamiczne są poddane pewnym globalnym więzom. Na tej podstawie otrzymano zarówno lokalne (makro-konstytutywne) jak i globalne (dotyczące całej struktury kompozytowej) modele obliczeniowe pewnych termo-niesprężystych kompozytów.

В работе представлен подход к термодынамике, в котором термодинамические процессы подвергнуты некоторым глобальным связям. На этой основе получены так локальные (макроопределяющие), как и глобальные (касающиеся целой композитной структуры) расчетные модели некоторых термо-неупругих композитов.

#### 1. Aim and scope of the contribution

THE AIM of this paper is twofold. Firstly, we formulate a general approach to thermodynamics of nonelastic materials which takes into account the constraints imposed on global processes. The proposed constrained thermodynamics makes it possible to produce in a consistent way different computational models for special problems and to develop engineering theories involving thermomechanical fields. Secondly, on the basis of constrained thermodynamics we also propose the method of a passage from micro- to macro-thermodynamics of certain inelastic materials. This method comprises two steps: (i) the local macro-modelling in which we deal with the fixed representative volume element (r.v.e.) of a body and we determine the averaged properties of a composite material, (ii) the global macro-modelling in which we obtain a macro-description of a whole composite body under consideration. It is assumed that the investigated composite bodies which are micro-nonhomogeneous by the definition may also be macro-nonhomogeneous and hence the known homogenization procedures [1, 6] cannot be applied. The proposed macro-modelling method can be treated as an alternative to the known methods based on the bounding principles or on the exact or approximate solutions, [2], including asymptotic approaches, [1, 3, 4, 6, 7] as well as non-standard analysis approaches, [8, 9], which have played an important role mainly in the macro-modelling of thermo-elastic composites. It will be shown that the main features of the proposed method are: 1) the method can be applied to an arbitrary dissipative heterogeneous material structure of the r.v.e.; 2) the method is effective from the engineering point of view; in particular no solution to the boundary value problem for the r.v.e. is required; 3) the method is adaptive and makes it possible to obtain different macro-models of composite materials on the different levels of accuracy. The main drawback of the proposed macro-modelling approach lies in the specification of constraints which is often guided by the physical institution of the researcher and in an ambiguous approximation introduced by the localization as-

sumption. For the sake of simplicity we restrict ourselves to the thermo-elastic and to the thermo-elastic-plastic materials with the perfect bonding between the adjacent constituent of the composite. The considerations are also carried out in the context of infinitesimal strains. It has to be emphasized, however, that the line of approach proposed in the contribution can also be applied to more general physical situations where we have to deal with the finite strains and imperfect bonding of adjacent materials.

Throughout the paper the subscripts i, j, ... run over 1, 2, 3 and the indices a, b, ... and A, B, ... run over 1, 2, ..., n and 1, 2, ..., N, respectively. The summation convention holds with respect to all aforementioned indices.

### 2. Introductory concepts

Let V be the regular region in 3-space occupied by the composite (or its part) in the referential configuration. Introducing the decomposition  $\overline{V} = M \cup I \cup \partial V$ , we denote by M the finite sum of disjoined regions occupied by the homogeneous components of the composite, by I the sum of interfaces between these regions and by  $\partial V$  the boundary of V; hence  $\partial M = I \cup \partial V$ . Let  $[\tau_0, \tau_f]$  be the known time interval and  $\psi(\tau) \equiv \psi(\cdot, \tau)$  stands for an arbitrary field defined on  $\overline{V}$ , M or  $\partial M$ , related to the time instant  $\tau \in [\tau_0, \tau_f]$ . We introduce the concept of the internal thermodynamical process as a sufficiently regular mapping

(2.1) 
$$[\tau_0, \tau_f] \ni \tau \to (\mathbf{u}(\tau), \theta(\tau), \sigma(\tau), \mathbf{h}(\tau), \varepsilon(\tau), \eta(\tau)),$$

where the fields on the right-hand side of Eq. (2.1) represent the states of displacement, absolute temperature, stress, heat flux, internal energy and specific entropy, respectively, at the time instant  $\tau$ . The field  $\mathbf{u}(\tau), \theta(\tau)$  are continuous and defined on  $\overline{V}$  and the fields  $\sigma(\tau), \mathbf{h}(\tau), \varepsilon(\tau), \eta(\tau)$  are defined on M. We also introduce the external action process

(2.2) 
$$[\tau_0, \tau_f] \ni \tau \to (\mathbf{f}(\tau), \mathbf{t}(\tau), \alpha(\tau), \beta(\tau)),$$

where  $\mathbf{f}(\tau)$ ,  $\alpha(\tau)$  are the total volume forces and heat sources defined on M and  $\mathbf{t}(\tau)$ ,  $\beta(\tau)$ are the total surface tractions and heat sources defined on  $\partial M$  (except possibly some lines or points on  $\partial M$ ), respectively, acting at the time instant  $\tau$ . Setting  $\mathbf{v}(\mathbf{y}, \tau) \equiv \dot{\mathbf{u}}(\mathbf{y}, \tau)$ ,  $\kappa(\mathbf{y}, \tau) \equiv (1/\theta(\mathbf{y}, \tau))$ ,  $\mathbf{y} \in \overline{V}$ , we define the velocity  $\mathbf{v}(\tau)$  and coolness rate  $\kappa(\tau)$  fields. The sets of all velocity fields and coolness rate fields constitute certain linear topological spaces which will be denoted by  $\mathcal{V}$  and  $\mathcal{K}$ , respectively. Let  $\mathcal{F}$  and  $\mathcal{H}$  stand for the sets of all force systems  $(\mathbf{f}, \mathbf{t})$  and heat source systems  $(\alpha, \beta)$ , respectively. To every  $(\mathbf{f}, \mathbf{t}) \in \mathcal{F}$ and every  $(\alpha, \beta) \in \mathcal{H}$  we shall assign the linear continuous functionals  $v^*(\mathbf{f}, \mathbf{t})$ ,  $\kappa^*(\alpha, \beta)$ defined on  $\mathcal{V}$  and  $\mathcal{K}$ , respectively, setting

(2.3) 
$$\langle \mathbf{v} || v^*(\mathbf{f}, \mathbf{t}) \rangle \equiv \int_M f_i(\mathbf{y}) v_i(\mathbf{y}) \, dy + \int_{\partial M} t_i(\mathbf{y}) v_i(\mathbf{y}) \, da \quad \text{for every} \quad \mathbf{v} \in \mathcal{V} ,$$
$$\langle \kappa | \kappa^*(\alpha, \beta) \rangle \equiv \int_M \alpha(\mathbf{y}) \kappa(\mathbf{y}) \, dy + \int_{\partial M} \beta(\mathbf{y}) \kappa(\mathbf{y}) \, da \quad \text{for every} \quad \kappa \in \mathcal{K} .$$

The functional  $\langle \cdot | v^*(\mathbf{f}, \mathbf{t}) \rangle$  represents the rate of work done by the force system  $(\mathbf{f}, \mathbf{t})$  while the functional  $\langle \cdot | \kappa^*(\alpha, \beta) \rangle$  can be interpreted as the entropy production rate done by the heat source system  $(\alpha, \beta)$ . It can be also observed that the set of all stress fields and the set of all heat flux fields constitute linear topological spaces which will be denoted by  $\mathcal{D}$ 

and  $\mathcal{G}$ , respectively. On these spaces we shall define the bilinear forms

(2.4) 
$$(\mathbf{d} \| \boldsymbol{\sigma}) \equiv \int_{M} d_{ij}(\mathbf{y}) \sigma_{ij}(\mathbf{y}) \, dy \,, \quad (\mathbf{g} | \mathbf{h}) \equiv \int_{M} g_i(\mathbf{y}) h_i(\mathbf{y}) \, dy \,.$$

We shall assume that for every  $\mathbf{v} \in \mathcal{V}$  and every  $\kappa \in \mathcal{K}$  there are defined the linear continuous operators  $L: \mathcal{V} \to \mathcal{D}$  and  $\nabla: \mathcal{K} \to \mathcal{G}$ , given by  $(L\mathbf{v})_{ij}(\mathbf{y}) \equiv v_{(i,j)}(\mathbf{y})$  and  $(\nabla \kappa)_i(\mathbf{y}) \equiv \kappa_{,i}(\mathbf{y}), \mathbf{y} \in M$ , respectively. Hence  $(L\mathbf{v}|\sigma)$  is a value of the stress power done by the stress field  $\sigma$  on the strain rate field  $L\mathbf{v}$ . Similarly,  $(\nabla \kappa | \mathbf{h})$  is a value of the entropy production rate done by the heat flux field  $\mathbf{h}$  on the coolness gradient field  $\nabla \kappa$ .

### 3. Fundamentals

Using the concepts introduced in Sect. 2 and denoting by  $\rho \dot{\mathbf{v}}(\tau)$ ,  $\rho \dot{\epsilon}(\tau)$  and  $\operatorname{tr}(\sigma L \mathbf{v})(\tau)$ the fields defined on M by means of  $\rho(\mathbf{y})\dot{v}_i(\mathbf{y},\tau)$ ,  $\rho(\mathbf{y})\dot{\epsilon}(\mathbf{y},\tau)$  and  $\sigma_{ij}(\mathbf{y})v_{(i,j)}(\mathbf{y})$ ,  $\mathbf{y} \in M$ , respectively, where  $\rho(\cdot)$  stands for the mass density in the referential state of the composite, we shall postulate the equations of motion and the energy balance equation in the following weak form:

(3.1) 
$$\begin{array}{l} (L\mathbf{v}||\boldsymbol{\sigma}(\tau)) = \langle \mathbf{v}||\boldsymbol{v}^{*}(\mathbf{f}(\tau) - \varrho\dot{\mathbf{v}}(\tau), \mathbf{t}(\tau))\rangle & \text{for every} \quad \mathbf{v} \in \mathcal{V}, \\ (\nabla\kappa|\mathbf{h}(\tau)) = \langle \kappa|\kappa^{*}(\alpha(\tau) - \varrho\dot{\varepsilon}(\tau) + \mathrm{tr}(\boldsymbol{\sigma} L\mathbf{v})(\tau), \beta(\tau))\rangle & \text{for every} \quad \kappa \in \mathcal{K}, \end{array}$$

which has to hold for an arbitrary  $\tau \in [\tau_0, \tau_f]$ .

In order to introduce the constitutive relations in the presence of the stress constraints (which will be investigated below), we postulate the following decompositions:

(3.2) 
$$v_{(i,j)}(\tau) = d_{ij}^C(\tau) + d_{ij}^R(\tau), \quad \eta(\tau) = \eta^C(\tau) + \eta^R(\tau), \quad \tau \in [\tau_0, \tau_f],$$

where the fields  $d_{ij}^C(\tau)$ ,  $\eta^C(\tau)$  will be called the constitutive strain rate field and the constitutive specific entropy field, respectively. The interpretation of the fields  $d_{ij}^R(\tau)$ ,  $\eta^R(\tau)$  will be given below. For the sake of simplicity we shall restrict ourselves to the elastic-plastic and elastic/viscoplastic materials which can be jointly defined by the constitutive relations of the form

(3.3)  

$$d_{ij}^{C}(\mathbf{y},\tau) = \widehat{d}_{ij}(\mathbf{y};\sigma(\mathbf{y},\tau),\dot{\sigma}(\mathbf{y},\tau),\theta(\mathbf{y},\tau),\dot{\theta}(\mathbf{y},\tau))$$

$$h_{i}(\mathbf{y},\tau) = k_{ij}(\mathbf{y};\theta(\mathbf{y},\tau))\theta_{,j}(\mathbf{y},\tau),$$

$$\varepsilon(\mathbf{y},\tau) = \varphi^{C}(\mathbf{y},\tau) + \theta(\mathbf{y},\tau)\eta^{C}(\mathbf{y},\tau),$$

$$\varphi^{C}(\mathbf{y},\tau) = \widehat{\varphi}(\mathbf{y};L\mathbf{u}(\mathbf{y},\tau),\theta(\mathbf{y},\tau)),$$

$$\eta^{C}(\mathbf{y},\tau) = \widehat{\eta}(\mathbf{y};L\mathbf{u}(\mathbf{y},\tau),\theta(\mathbf{y},\tau)), \quad \mathbf{y} \in M.$$

For every special class of materials the constitutive functions on the right-hand sides of Eqs. (3.3) have to be specified. In particular, for elastic/viscoplastic materials we get

(3.4) 
$$d_{ij}^{C}(\mathbf{y},\tau) = a_{ijkl}(\mathbf{y};\theta(\mathbf{y},\tau))\dot{\sigma}_{kl}(\mathbf{y},\tau) + b_{ij}(\mathbf{y};\theta(\mathbf{y},\tau))\dot{\theta}(\mathbf{y},\tau) + \partial\gamma(\mathbf{y};\sigma(\mathbf{y},\tau),\theta(\mathbf{y},\tau))/\partial\sigma_{ij}(\mathbf{y},\tau)$$

and for elastic-plastic materials we assume

(3.5) 
$$d_{ij}^{C}(\mathbf{y},\tau) = a_{ijkl}^{EP}(\mathbf{y};\sigma(\mathbf{y},\tau),\dot{\sigma}(\mathbf{y},\tau)), \theta(\mathbf{y},\tau))\dot{\sigma}_{kl}(\mathbf{y},\tau) + b_{ij}^{EP}(\mathbf{y};\sigma(\mathbf{y},\tau),\dot{\sigma}(\mathbf{y},\tau),\theta(\mathbf{y},\tau))\dot{\theta}(\mathbf{y},\tau),$$

where the form of functions  $a_{ijkl}^{EP}(\mathbf{y}; \cdot)$ ,  $b_{ij}^{EP}(\mathbf{y}; \cdot)$ ,  $\gamma(\mathbf{y}; \cdot)$  can be found in the recent literature on this subject.

The constitutive relations have to be considered together with the known dissipation inequality

(3.6) 
$$\varrho(\mathbf{y})[\dot{\eta}(\mathbf{y},\tau) - \dot{\varepsilon}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau)] + \sigma_{ij}(\mathbf{y},\tau)v_{(i,j)}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau) + h_i(\mathbf{y},\tau)\theta_{,i}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau)^2 \ge 0$$

which has to hold for every  $\mathbf{y} \in M$  and  $\tau \in [\tau_0, \tau_f]$ .

Now we introduce the concept of loadings by assuming that in the problem under consideration for every  $\tau \in [\tau_0, \tau_f]$  the relation  $\mathcal{L}_{\tau} \subset \mathcal{F} \times \mathcal{H}$  is known. An arbitrary (sufficiently regular) mapping  $[\tau_0, \tau_f] \ni \tau \to (\mathbf{f}^L(\tau), \mathbf{t}^L(\tau), \alpha^L(\tau), \beta^L(\tau))$  satisfying the condition

(3.7) 
$$(\mathbf{f}^{L}(\tau), \mathbf{t}^{L}(\tau), \alpha^{L}(\tau), \beta^{L}(\tau)) \in \mathcal{L}_{\tau}, \quad \tau \in [\tau_{0}, \tau_{f}],$$

will be interpreted as a (mechanical and thermal) loading process of composite. The relation (3.7) for any  $\tau \in [\tau_0, \tau_f]$  will be referred to as the loading relation.

REMARK. In many problems (which will not be investigated here) the sets  $\mathcal{L}_{\tau}$  are singletons uniquely determined by the fields  $\mathbf{u}(\tau), \theta(\tau), \dot{\mathbf{u}}(\tau), \dot{\theta}(\tau)$ ).

Passing to the concept of the global constraints, we shall postulate that to arbitrary displacement **u** and absolute temperature  $\theta$  fields at every  $\tau \in [\tau_0, \tau_f]$  there are assigned the known (possibly empty) closed convex sets  $\mathcal{V}_{\tau}(\mathbf{u}), \mathcal{K}_{\tau}(\theta)$  in the linear topological spaces  $\mathcal{V}, \mathcal{K}$ , respectively. If the fields **u** and  $\theta$  cannot be realized at a time instant  $\tau$ , then  $\mathcal{V}_{\tau}(\mathbf{u}) = \phi$  and  $\mathcal{K}_{\tau}(\theta) = \phi$ . We shall also postulate that the closed convex nonempty set  $\mathcal{D}_0$  in the linear topological space  $\mathcal{D}$  of all stress fields is known. Under foregoing notations we shall assume that in the problem considered only such internal thermodynamical processes (2.1) can be realized which satisfy the conditions

(3.8)  $\mathbf{v}(\tau) \in \mathcal{V}_{\tau}(\mathbf{u}(\tau)), \quad \kappa(\tau) \in \mathcal{K}_{\tau}(\theta(\tau)), \quad \sigma(\tau) \in \mathcal{D}_{0}, \quad \tau \in [\tau_{0}, \tau_{f}].$ 

The above formulae will be referred to as the global (thermomechanical) constraints.

REMARK. In more general situation, which will be investigated elsewhere, we also have to introduce the heat flux constraints  $\mathbf{h}(\tau) \in \mathcal{G}_0$  where  $\mathcal{G}_0$  is the known closed convex and nonempty subset in the linear topological space  $\mathcal{G}$ .

The concept of constraints is closely related to the notion of reactions which maintain the above constraints. For the known loading process  $\tau \to (\mathbf{f}^L(\tau), \mathbf{t}^L(\tau), \alpha^L(\tau), \beta^L(\tau))$  and an arbitrary external action process (2.1), define

(3.9) 
$$(\mathbf{f}^{R}(\tau), \mathbf{t}^{R}(\tau), \alpha^{R}(\tau), \beta^{R}(\tau))$$
  

$$\equiv (\mathbf{f}(\tau) - \mathbf{f}^{L}(\tau), \mathbf{t}(\tau) - \mathbf{t}^{L}(\tau), \alpha(\tau) - \alpha^{L}(\tau), \beta(\tau) - \beta^{L}(\tau)).$$

Then the force system  $(\mathbf{f}^R(\tau), \mathbf{t}^R(\tau))$  will be interpreted as the reaction maintaining kinematical constraints  $\mathbf{v}(\tau) \in \mathcal{V}_{\tau}(\mathbf{u}(\tau))$  and the heat source system  $(\alpha^R(\tau), \beta^R(\tau))$  will stand for the reaction to the thermal constraints  $\kappa(\tau) \in \mathcal{K}_{\tau}(\theta(\tau))$ . The aforementioned reactions will be termed perfect if the following minimum conditions hold in  $[\tau_0, \tau_f]$ :

(3.10) 
$$\frac{\langle \mathbf{v} || v^*(\mathbf{f}^R(\tau), \mathbf{t}^R(\tau)) \rangle \geq \langle \mathbf{v}(\tau) || v^*(\mathbf{f}^R(\tau), \mathbf{t}^R(\tau)) \rangle \quad \text{for every} \quad \mathbf{v} \in \mathcal{V}_{\tau}(\mathbf{u}(\tau)), \\ \langle \kappa | \kappa^*(\alpha^R(\tau), \beta^R(\tau)) \rangle \geq \langle \kappa(\tau) | \kappa^*(\alpha^R(\tau), \beta^R(\tau)) \rangle \quad \text{for every} \quad \kappa \in \mathcal{K}_{\tau}(\theta(\tau)).$$

Remembering the decompositions (2.3), we shall interpret the fields  $\mathbf{d}^{R}(\tau)$ ,  $\eta^{R}(\tau)$  as the reactions to the stress constraints  $\sigma(\tau) \in \mathcal{D}_{0}$ . These reactions will be called perfect if the following maximum conditions hold in  $[\tau_{0}, \tau_{f}]$ :

(3.11) 
$$(\sigma \| \mathbf{d}^R(\tau)) \le (\sigma(\tau) \| \mathbf{d}^R(\tau))$$
 for every  $\sigma \in \mathcal{D}_0$ ,

and if the entropy production due to the reactions  $\mathbf{d}^{R}(\tau)$ ,  $\eta^{R}(\tau)$  is equal to zero; by means of the inequality (3.6) we have

(3.12) 
$$\varrho(\mathbf{y})\dot{\eta}^{R}(\mathbf{y},\tau) + \sigma_{ij}(\mathbf{y},\tau)d_{ij}^{R}(\mathbf{y},\tau) = 0, \quad \mathbf{y} \in M, \quad \tau \in [\tau_{0},\tau_{f}].$$

In the sequel we shall deal exclusively with the perfect reactions to the constraints (3.8). The physical interpretation of the conditions (3.10) and (3.11) can be easily derived from the interpretation of the pertinent functionals which were introduced in Sect. 2.

The variational field equations (3.1), constitutive relations (3.3), dissipation inequality (3.6), loading relations (3.7), constraint relations (3.8), reaction relations (3.10)–(3.12) and decompositions (3.2) and (3.9) represent the fundamentals of thermodynamics with the global (or field) constraints.

#### 4. Governing relations

Using the relations (3.2), (3.9), (3.1) and (3.10), we can eliminate the reactions  $(\mathbf{f}^R(\tau), \mathbf{t}^R(\tau), \alpha^R(\tau), \beta^R(\tau))$  from the system of relations introduced in Sect. 3.

This way we arrive at the conditions

(4.1)  

$$(L\mathbf{v} - L\mathbf{v}(\tau) || \boldsymbol{\sigma}(\tau)) \geq \langle \mathbf{v} - \mathbf{v}(\tau) || v^{*} (\mathbf{f}^{L}(\tau) - \varrho \dot{\mathbf{v}}(\tau), \mathbf{t}^{L}(\tau)) \rangle$$

$$(\nabla \kappa - \nabla \kappa(\tau) |\mathbf{h}(\tau)\rangle \geq \langle \kappa - \kappa(\tau) | \kappa^{*} (\alpha^{L}(\tau) - \varrho \dot{\varepsilon}(\tau) + \operatorname{tr}(\boldsymbol{\sigma} L\mathbf{v})(\tau), \beta^{L}(\tau)) \rangle$$
for every  $\kappa \in \mathcal{K}_{\tau}(\theta(\tau))$ .

for  $\tau \in [\tau_0, \tau_f]$ . Similarly, using the relations (3.11) and (3.2), we can eliminate the reactions  $\mathbf{d}^R(\tau)$ . Hence

(4.2) 
$$(\boldsymbol{\sigma} - \boldsymbol{\sigma}(\tau) \| L \mathbf{v}(\tau)) \leq (\boldsymbol{\sigma} - \boldsymbol{\sigma}(\tau) \| \mathbf{d}^{C}(\tau))$$
 for every  $\boldsymbol{\sigma} \in \mathcal{D}_{0}$ ,

for  $\tau \in [\tau_0, \tau_f]$ . The conditions (4.1) will be called the virtual power principle and virtual entropy production rate principle. Similarly, the condition (4.2) will be referred to as the complementary power principle. At the same time from the relations (3.6) and (3.12) we get

(4.3) 
$$\varrho(\mathbf{y})[\dot{\eta}^{C}(\mathbf{y},\tau) - \dot{\varepsilon}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau)] + \sigma_{ij}(\mathbf{y},\tau)d_{ij}^{C}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau) + h_{i}(\mathbf{y},\tau)\theta_{,i}(\mathbf{y},\tau)/\theta(\mathbf{y},\tau)^{2} \ge 0 , \quad \mathbf{y} \in M ,$$

for  $\tau \in [\tau_0, \tau_f]$ . According to the line of approach of rational thermodynamics, we shall assume that the inequality (4.3) has to be identically satisfied by the constitutive functions  $\hat{d}_{ij}(y; \cdot), k_{ij}(\mathbf{y}; \cdot), \hat{\varphi}(y; \cdot)$  and  $\hat{\eta}(y; \cdot)$  on the right-hand sides of Eqs. (3.3).

Summarizing the obtained results, we conclude that the governing relations of the constrained thermodynamics (under the assumptions introduced above) are given by: (i) virtual power principle and virtual entropy production rate principle (4.1), (ii) complementary power principle (4.2), (iii) constraint relations (3.8), (iv) loading relations (3.7), (v) constitutive relations (3.3) which have to be restricted by the dissipation inequality (4.3).

#### 5. Special constraints

Define  $\mathcal{U}_{\tau} = \{\mathbf{u} : \mathcal{V}_{\tau}(u) \neq \phi\}, \mathcal{T}_{\tau} = \{\theta : \mathcal{K}_{\tau}(\theta) \neq \phi\}$  for every  $\tau \in [\tau_0, \tau_f]$  and assume that

(5.1) 
$$\mathbf{u}(\tau) \in \mathcal{U}_{\tau}, \quad \theta(\tau) \in \mathcal{T}_{\tau}, \quad \boldsymbol{\sigma}(\tau) \in \mathcal{D}_{0}, \quad \tau \in [\tau_{0}, \tau_{f}],$$

imply the constraint relations (3.8). In this case the kinematical and thermal constraints will be referred to as the configurational constraints.

Let  $\mathcal{V}(\mathbf{u}; \tau), \mathcal{K}(\theta; \tau)$ , for every  $\tau \in [\tau_0, \tau_f]$  and every  $\mathbf{u} \in \mathcal{U}_{\tau}, \theta \in \mathcal{T}_{\tau}$ , be the closed non-empty linear subspaces in the linear spaces  $\mathcal{V}, \mathcal{K}$ , respectively. Let us also assume that  $\mathcal{V}_{\tau}(\mathbf{u}) = \mathcal{V}(\mathbf{u}; \tau) + \mathbf{v}, \mathcal{K}_{\tau}(\theta) = \mathcal{K}(\theta; \tau) + \kappa$  for arbitrary  $\mathbf{v} \in \mathcal{V}_{\tau}(\mathbf{u}), \kappa \in \mathcal{K}_{\tau}(\theta)$ ; this means that every non-empty set  $\mathcal{V}_{\tau}(\mathbf{u})$  and  $\mathcal{K}_{\tau}(\theta)$  represent a certain linear manifold in  $\mathcal{V}$  and  $\mathcal{K}$ , respectively. Under this assumption the virtual power principle and the virtual entropy production rate principle (4.1) reduce to

(5.2) 
$$\begin{aligned} (L\mathbf{v}||\boldsymbol{\sigma}(\tau)) &= \langle \mathbf{v}||v^*(\mathbf{f}^L(\tau) - \varrho\dot{\mathbf{v}}(\tau), \mathbf{t}^l(\tau)) \rangle & \text{for every} \quad \mathbf{v} \in \mathcal{V}(\mathbf{u}(\tau); \tau) , \\ (\nabla\kappa|\mathbf{h}(\tau)) &= \langle \kappa|\kappa^*(\alpha^L(\tau) - \varrho\dot{\varepsilon}(\tau) + \operatorname{tr}(\boldsymbol{\sigma} L\mathbf{v})(\tau), \beta^L(\tau)) \rangle \\ & \text{for every} \quad \kappa \in \mathcal{K}(\theta(\tau); \tau) , \end{aligned}$$

for every  $\tau \in [\tau_0, \tau_f]$ . In this case the kinematical and thermal constraints will be called bilateral. Similarly, assume that  $\mathcal{D}_0$  is the closed non-empty linear subspace in the linear space  $\mathcal{D}$ . Then the complementary power principle (4.2) will take the form

(5.3) 
$$(\sigma || L\mathbf{v}(\tau)) = (\sigma || \mathbf{d}^C(\tau))$$
 for every  $\sigma \in \mathcal{D}_0$ 

and the stress constraints will be called bilateral.

#### 6. Local macro-modelling

In the local macro-modelling we restrict ourselves to the investigation of thermodynamics in a certain arbitrary but fixed representative volume element of the composite structure under consideration. The analysis will be based on the relations of constrained thermodynamics, summarized in Sect. 4; the foundations of the modelling reduce to the specification of the constraint relations (3.8) and loading relations (3.7) and to the following:

LOCALIZATION ASSUMPTION. The relations of macro-thermodynamics have to be invariant under arbitrary rescalling  $V \rightarrow \varepsilon V$ ,  $\varepsilon \in (0, 1)$ , of every representative volume element of the composite structure.

The forementioned assumption is motivated by the fact that the macro-modelling procedure has a physical sense only if the maximum length dimension of the r.v.e. is negligibly small as compared to all length dimensions related to the problem for the whole composite structure. It follows that from the computational point of view the r.v.e. has to be treated as infinitely small; hence the methods of the nonstandard analysis can be used as a tool of modelling, see [8].

Let V be the neighbourhood of the point y = 0 in  $\mathbb{R}^3$ . We shall specify the configura-

tional constraints (5.1) by assuming that

$$u_{i}(\mathbf{y},\tau) = U_{i}(\tau) + F_{ij}(\tau)y_{j} + l_{a}(\mathbf{y})U_{i}^{a}(\tau), \quad \mathbf{y} \in \overline{V},$$

$$(6.1) \qquad c(\mathbf{y},\tau) \equiv \theta(\mathbf{y},\tau)^{-1} = C(\tau) + C_{i}(\tau)y_{i} + l_{a}(\mathbf{y})C^{a}(\tau), \quad \mathbf{y} \in \overline{V},$$

$$\sigma_{ij}(\mathbf{y},\tau) = S_{ij}^{0} + m_{Aijkl}(\mathbf{y})S_{kl}^{A}(\tau), \quad \mathbf{y} \in M, \quad \tau \in [\tau_{0},\tau_{f}],$$

where  $l_a(\cdot)$ ,  $m_{Aijkl}(\cdot)$  are postulated *a priori* (in every special problem) shape functions and  $U_i(\cdot)$ ,  $F_{ij}(\cdot)$ ,  $U_i^a(\cdot)$ ,  $C(\cdot)$ ,  $C_i(\cdot)$ ,  $C^a(\cdot)$ ,  $S_{ij}^0(\cdot)$ ,  $S_{ij}^A(\cdot)$  are arbitrary sufficiently regular functions called macro-parameters. We also assume that  $S_{ij}^0(\mathbf{y}) = S_{ji}^0(\mathbf{y})$ ,  $S_{ij}^A(\mathbf{y}) = S_{ii}^A(y)$  and

$$det[\delta_{ij} + F_{ij}(\tau)] > 0, \qquad \int_{V} l_{a,i}(\mathbf{y}) \, dy = 0, \qquad m_{Aijkl}(\mathbf{y}) = m_{Aklij}(\mathbf{y})$$

and that the shape functions are independent.

The specification of the loading relation (3.7) will be assumed in the form

(6.2) 
$$\begin{aligned} f_i^L(\mathbf{y},\tau) &= \varrho(\mathbf{y})b_i(\mathbf{y},\tau), \quad \mathbf{y} \in M, \quad t_i^L(\mathbf{y},\tau) = 0, \quad \mathbf{y} \in I, \\ t_i^L(\mathbf{y},\tau) &= (T_{ij}(\tau) + T_{ijk}(\tau)y_k)n_j(\mathbf{y}), \quad \mathbf{y} \in \partial V, \quad T_{ijk}(\tau) = 0 \quad \text{if} \quad j \neq k, \\ \alpha^L(\mathbf{y},\tau) &= \varrho(\mathbf{y})\zeta(\mathbf{y},\tau), \quad \mathbf{y} \in M, \quad \beta^L(\mathbf{y},\tau) = 0, \quad \mathbf{y} \in I, \\ \beta^L(\mathbf{y},\tau) &= (H_i(\tau) + H_{ij}(\tau)y_j)n_i(\mathbf{y}), \quad \mathbf{y} \in \partial V, \quad H_{ik}(\tau) = 0 \quad \text{if} \quad i \neq k, \end{aligned}$$

where  $n_i(\mathbf{y})$  is a unit normal outward to  $\partial V$ , the functions  $\varrho(\cdot), b_i(\cdot), \zeta(\cdot)$  are known in every problem under consideration and  $T_{ij}(\cdot), H_i(\cdot), T_{ijk}(\cdot), H_{ij}(\cdot)$  are arbitrary sufficiently regular functions.

The specifications of constraints (6.1) and loadings (6.2) together with the localization assumption make it possible to determine the averaged thermodynamics of the r.v.e. To this end we introduce the well-known mean value operator

(6.3) 
$$\langle \psi \rangle = \langle \psi \rangle (\Xi) = \frac{1}{\operatorname{vol} V} \int_{V} \psi(\mathbf{y}, \Xi) \, dy$$

where  $\psi(\cdot)$  is an arbitrary integrable function and  $\Xi$  is a finite sequence of parameters which are independent of  $\mathbf{y} \in V$ .

Using Eqs. (6.1) and (6.2), from the virtual power principle (5.2) we obtain

(6.4)  

$$T_{ikk}(\tau) + \langle \varrho b_i \rangle(\tau) = \langle \varrho \rangle U_i(\tau) ,$$

$$T_{ij}(\tau) = S_{ij}^0(\tau) + \langle m_{Aijkl} \rangle S_{kl}^A(\tau) ,$$

$$\langle l_{a,j} m_{Aijkl} \rangle S_{kl}^A(\tau) = 0 .$$

Similarly, from Eqs. (6.1) and (6.2) and the virtual entropy production rate principle (5.2), we get

(6.5) 
$$\overline{\langle \varrho \varepsilon \rangle}(\tau) = H_{ii}(\tau) + T_{ij}(\tau) \dot{E}_{ij}(\tau) + \langle \varrho \zeta \rangle(\tau), \quad E_{ij} = F_{(ji)}.$$

At last, the complementary power principle (5.3) and the condition (6.2) for the stress components yield

(6.6) 
$$\begin{aligned} E_{ij}(\tau) &= \langle d_{ij}^C \rangle(\tau) , \quad D_{Aij}(\tau) &= \langle m_{Aijkl} d_{kl}^C \rangle(\tau) , \\ \langle m_{Aijkl} \rangle \dot{E}_{kl}(\tau) &+ \langle m_{Aijkl} l_{a,k} \rangle \dot{U}_l^a(\tau) &= D_{Aij}(\tau) . \end{aligned}$$

In order to obtain the averaged form of the dissipation inequality (4.3), we introduce the denotations

(6.7) 
$$\Theta(\tau) \equiv C(\tau)^{-1}, \quad G_i(\tau)^{-1} \equiv -C_i(\tau)\Theta(\tau)^2, \quad G^a(\tau) \equiv -C^a(\tau)\Theta(\tau)^2,$$

and we take into account Eqs. (6.1) and (6.2). Hence

(6.8) 
$$\overline{\langle \varrho \eta^C \rangle} - \overline{\langle \varrho \varepsilon \rangle} / \Theta + S^0_{ij} \dot{E}_{ij} / \Theta + S^A_{ij} D_{Aij} / \Theta + H_i G_i / \Theta^2 = 0.$$

It has to be emphasized that Eqs. (6.4)–(6.6) and the inequality (6.8) as well as all subsequent relations of the averaged thermodynamics of the r.v.e. are obtained under the localization assumption, i.e., we reject all terms of an order of the length dimensions of  $\overline{V}$ . It can also be shown that the following formulae hold true:

(6.9) 
$$T_{ij} = \langle \sigma_{ij} \rangle, \quad T_{ikk} = \langle \sigma_{ik,k} \rangle - \frac{1}{\operatorname{vol}V} \int_{I} \left[ [\sigma_{ik}] n_k \, da \,, \quad \langle \sigma_{ij} l_{a,j} \rangle = 0 \,,$$
$$H_i = \langle h_i \rangle, \quad H_{ii} = \langle h_{i,i} \rangle - \frac{1}{\operatorname{vol}V} \int_{I} \left[ [h_i] n_i \, da \,, \qquad \langle h_i l_{a,i} \rangle = 0 \,,$$
$$T_{ij} \dot{E}_{ij} = \langle \sigma_{ij} v_{(i,j)} \rangle \,.$$

All the formulae derived above are independent of the material properties of the r.v.e. Now, taking into account the constitutive relations in their general form (3.3), from Eqs. (6.6) we obtain immediately

(6.10) 
$$\begin{split} \dot{E}_{ij} &= \langle \hat{d}_{ij} \rangle (\mathbf{S}, \mathbf{S}^0, \dot{\mathbf{S}}, \dot{\mathbf{S}}^0, \Theta, \dot{\Theta}) , \quad \mathbf{S} \equiv \{\mathbf{S}^1, \dots, \mathbf{S}^N\} , \\ D_{Aij} &= \langle m_{Aijkl} \hat{d}_{kl} \rangle (\mathbf{S}, \mathbf{S}^0, \dot{\mathbf{S}}, \dot{\mathbf{S}}^0, \Theta, \dot{\Theta}) . \end{split}$$

From the constitutive relations (3.3) for the heat flux  $h_i(\mathbf{y}, \tau)$  and from the formulae (6.9) we get

(6.11) 
$$H_i = \langle k_{ij} \rangle G_j + \langle k_{ij} l_{a,j} \rangle G^a ,$$
$$0 = \langle k_{ij} l_{a,i} \rangle G_j + \langle l_{a,i} k_{ij} l_{b,j} \rangle G^b , \quad k_{ij} = k_{ij} (\mathbf{y}, \Theta) .$$

At last, the constitutive relations (3.3) for the internal energy yield

(6.12) 
$$\begin{array}{l} \langle \varrho \varepsilon \rangle = \langle \varrho \varphi^C \rangle + \Theta \langle \varrho \eta^C \rangle , \\ \langle \varrho \varphi^C \rangle = \langle \varrho \widehat{\varphi} \rangle (\mathbf{E}, \mathbf{U}, \Theta) , \quad \langle \varrho \eta^C \rangle = \langle \varrho \widehat{\eta} \rangle (\mathbf{E}, \mathbf{U}, \Theta) , \quad \mathbf{U} \equiv \{ \mathbf{U}^1, \dots, \mathbf{U}^n \} . \end{array}$$

It has to be emphasized that the averaged constitutive relations (6.10)–(6.12) were obtained with the aid of the constraint relations (6.1) and under the denotations (6.7).

So far, no restrictions were imposed on the form of the constraints (6.1); hence some unphysical situations may take place if the shape functions in Eqs. (6.1) are not properly chosen. To avoid such situations, we introduce the following:

DEFINITION. The constraints (6.1) are said to be well posed (for a class of thermo-elastoinelastic materials under consideration) if the material homogeneity of the r.v.e. and the uniform distribution of the inelastic part of the constitutive strain rate in the r.v.e. at every  $\tau \in [\tau_0, \tau_f]$  imply the uniform distribution of the displacement gradients  $u_{i,j}(\mathbf{y}, \tau)$ , temperature gradients  $\theta_{,i}(\mathbf{y}, \tau)$  and stresses  $\sigma_{ij}(\mathbf{y}, \tau)$  at every  $\tau \in [\tau_0, \tau_f]$ , provided that  $U_i^a(\mathbf{y}, \tau_0) = 0$ ,  $S_{ij}^A(\mathbf{y}, \tau_0) = 0$ ,  $\mathbf{y} \in M$ .

It has not be noted that the materials defined by the constitutive relations of the form (3.3) are called thermo-elasto-inelastic if

(6.13) 
$$d_{ij}^C(\mathbf{y},\tau) = a_{ijkl}(\mathbf{y};\theta(\mathbf{y},\tau))\dot{\sigma}_{kl}(\mathbf{y},\tau) + b_{ij}(\mathbf{y};\theta(\mathbf{y},\tau))\dot{\theta}(\mathbf{y},\tau) + n_{ij}(\mathbf{y},\tau), \quad \mathbf{y} \in M,$$

where the tensors  $a_{ijkl}(\mathbf{y}; \cdot), b_{ij}(\mathbf{y}; \cdot)$  describe the elastic properties of a material and

(6.14) 
$$n_{ij}(\mathbf{y},\tau) = \hat{n}_{ij}(\mathbf{y};\boldsymbol{\sigma}(\mathbf{y},\tau), \dot{\boldsymbol{\sigma}}(\mathbf{y},\tau), \theta(\mathbf{y},\tau), \dot{\theta}(\mathbf{y},\tau))$$

is the inelastic part of the strain rate tensor; the functions  $\hat{n}_{ij}(\mathbf{y}; \cdot)$  can also depend on the hardening parameters not specified here. We also have to remember that using the constraints (6.1), we tacitly assume that the localization assumption holds true, i.e., we neglect all terms of an order of the length dimensions of the r.v.e.

In the sequel we shall use the matrix notation, representing a symmetric tensor  $d_{ij} = d_{ji}$  by a column matrix  $\mathbf{d} = \{d_{11}, d_{22}, d_{33}, d_{12}, d_{23}, d_{31}\}^T$  and a tensor  $m_{ijkl}$ , such that  $m_{ijkl} = m_{jikl} = m_{jilk}$ , by  $6 \times 6$  matrix  $\mathbf{m} = [\mathbf{m}]_{6 \times 6}$ . Moreover, any product of the form  $g_i m_{ijkl}$ , where  $g_i$  is an arbitrary vector, will be represented by  $3 \times 6$  matrix denoted by  $\mathbf{gm} = [\mathbf{gm}]_{3 \times 6}$ .

PROPOSITION. The constraints (6.1) are well posed if the block matrix  $[\langle \mathbf{m}_A \mathbf{a} \mathbf{m}_B \rangle - \langle \mathbf{m}_A \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} \langle \mathbf{a} \mathbf{m}_B \rangle]$  has an inverse denoted by  $[\mathbf{B}^{AB}]_{6N \times 6N}$  and the block matrices  $[\langle \nabla l_a \mathbf{m}_A \rangle \mathbf{B}^{AB} \langle \mathbf{m}_B \nabla l_b \rangle]_{3n \times 3n}$ ,  $[\langle \nabla l_a \mathbf{k} \nabla l_b \rangle]_{n \times n}$  are non-singular.

Let  $[\mathbf{A}^{ab}]_{3n \times 3n}$  and  $[F^{ab}]_{n \times n}$  stand for the block matrices which are inverse to  $[\langle \nabla l_a \mathbf{m}_A \rangle \mathbf{B}^{AB} \langle \mathbf{m}_B \nabla l_b \rangle]$  and  $[\langle \nabla l_a \mathbf{k} \nabla l_b \rangle]$ , respectively. Then, from Eqs. (6.13), (6.6) and (6.4)<sub>3</sub> we obtain

$$\dot{\mathbf{S}}^{A} = \mathbf{B}^{AB}(\langle \mathbf{m}_{B} \nabla l_{a} \rangle \dot{\mathbf{U}}^{a} + (\langle \mathbf{m}_{B} \rangle - \langle \mathbf{m}_{B} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1}) \dot{\mathbf{E}} + \langle \mathbf{m}_{B} \rangle \langle \mathbf{a} \rangle^{-1} \langle \widetilde{\mathbf{n}} \rangle - \langle \mathbf{m}_{B} \widetilde{\mathbf{n}} \rangle),$$
(6.15) 
$$\dot{\mathbf{U}}^{a} = \mathbf{A}^{ab} \langle \nabla l_{b} \mathbf{m}_{B} \rangle \mathbf{B}^{BA}((\langle \mathbf{m}_{A} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} - \langle \mathbf{m}_{A} \rangle) \dot{\mathbf{E}} + \langle \mathbf{m}_{A} \widetilde{\mathbf{n}} \rangle - \langle \mathbf{m}_{A} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} \langle \widetilde{\mathbf{n}} \rangle),$$

$$G^{a} = -F^{ab} \langle \nabla l_{b} \mathbf{k} \rangle \cdot \mathbf{G}, \qquad \widetilde{n}_{ij} = n_{ij} + b_{ij} \dot{\theta},$$

provided that the conditions in the above proposition are satisfied. Bearing in mind the definition of the well-posed constraints and the condition  $\langle \nabla l_b \rangle = 0$ , for the homogeneous material structure of the r.v.e. and the uniform distribution of  $\mathbf{n}(\cdot, \tau)$ , under the localization assumption, we obtain from Eqs. (6.15) that  $\dot{\mathbf{S}}^A = \mathbf{0}$ ,  $\dot{\mathbf{U}}^a = \mathbf{0}$  and  $G^a = 0$ . Hence we conclude that the above proposition holds true.

COROLLARY. For the well-posed constraints the macro-heat flux  $H_i$  is related to the macro-temperature gradient  $G_j$  by means of

(6.16) 
$$H_i = (\langle k_{ij} \rangle - \langle k_{ik} l_{a,k} \rangle F^{ab} \langle l_{b,l} k_{lj} \rangle) G_j .$$

In the sequel we tacitly assume that the constraints (6.1) for the class of thermo-elastoinelastic materials under consideration are well posed.

Now assume that the material of the r.v.e. is thermo-elastic/viscoplastic. From Eqs. (3.4) and (6.13) we obtain

(6.17) 
$$n_{ij}(\mathbf{y},\tau) = \partial \gamma(\mathbf{y};\boldsymbol{\sigma}(\mathbf{y},\tau),\theta(\mathbf{y},\tau))/\partial \sigma_{ij}(\mathbf{y},\tau).$$

Eliminating  $\dot{U}^a$  from Eq. (6.15)<sub>1,2</sub> and using Eq. (6.17), after the denotation

(6.18) 
$$\begin{aligned} \widetilde{\mathbf{B}}^{AB} &\equiv \mathbf{B}^{AB} - \mathbf{B}^{AC} \langle \mathbf{m}_{C} \nabla l_{a} \rangle \mathbf{A}^{ab} \langle \nabla l_{b} \mathbf{m}_{D} \rangle \mathbf{B}^{DB} , \quad \mathbf{G}^{A} &\equiv \widetilde{\mathbf{B}}^{AB} \langle \mathbf{m}_{B} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} , \\ \mathbf{D}^{A} &\equiv \widetilde{\mathbf{B}}^{AB} (\langle \mathbf{m}_{B} \rangle - \langle \mathbf{m}_{B} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1}) , \quad \mathbf{B}^{A} &\equiv \widetilde{\mathbf{B}}^{AB} (\langle \mathbf{m}_{B} \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} \langle \mathbf{b} \rangle - \langle \mathbf{m}_{B} \mathbf{b} \rangle) , \end{aligned}$$

we obtain

(6.20)

(6.19) 
$$\dot{\mathbf{S}}^{A}(\tau) = \mathbf{D}^{A}\dot{\mathbf{E}}(\tau) + \mathbf{B}^{A}\dot{\Theta}(\tau) + \mathbf{G}^{A}\partial\langle\gamma\rangle/\partial\mathbf{S}^{0}(\tau) - \widetilde{\mathbf{B}}^{AB}\partial\langle\gamma\rangle/\partial\mathbf{S}^{B}(\tau).$$

Combining Eqs. (6.6)1, (6.13) and (6.1) and denoting

$$\begin{split} \mathbf{A} &\equiv \langle \mathbf{a} \rangle - (\langle \mathbf{a} \mathbf{m}_A \rangle - \langle \mathbf{a} \rangle \langle \mathbf{m}_A \rangle) \widetilde{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \mathbf{a} \rangle - \langle \mathbf{m}_B \rangle \langle \mathbf{a} \rangle) \,, \\ \mathbf{B} &\equiv \langle \mathbf{b} \rangle + (\langle \mathbf{a} \mathbf{m}_A \rangle - \langle \mathbf{a} \rangle \langle \mathbf{m}_A \rangle) \widetilde{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} \langle \mathbf{b} \rangle - \langle \mathbf{m}_B \mathbf{b} \rangle) \,, \\ \mathbf{C} &\equiv \mathbf{1} + (\langle \mathbf{a} \mathbf{m}_A \rangle - \langle \mathbf{a} \rangle \langle \mathbf{m}_A \rangle) \widetilde{\mathbf{B}}^{AB} \langle \mathbf{m}_B \mathbf{a} \rangle \langle \mathbf{a} \rangle^{-1} \,, \end{split}$$

$$\mathbf{C}^{A} \equiv (\langle \mathbf{a}\mathbf{m}_{B} \rangle - \langle \mathbf{a} \rangle \langle \mathbf{m}_{B} \rangle) \widetilde{\mathbf{B}}^{BA}$$

under the assumption that the  $6 \times 6$  matrix A is non-singular, we get

(6.21) 
$$\dot{\mathbf{E}}(\tau) = \langle \mathbf{a} \rangle \mathbf{A}^{-1} \langle \mathbf{a} \rangle \dot{\mathbf{T}}(\tau) + \langle \mathbf{a} \rangle \mathbf{A}^{-1} (\mathbf{B} \dot{\Theta}(\tau) + \mathbf{C} \partial \langle \gamma \rangle / \partial \mathbf{S}^{0}(\tau) + \mathbf{C}^{A} \partial \langle \gamma \rangle / \partial \mathbf{S}^{A}(\tau)) .$$

It is to remembered that the matrices defined by Eqs. (6.18) and (6.20) depend on the macro-temperature  $\Theta$ , and the averaged potential  $\langle \gamma \rangle$  is a function of the macro-parameters  $\mathbf{S}^0$ ,  $\mathbf{S} = \{S^1, \ldots, S^N\}$  and  $\Theta$ . At the same time  $\mathbf{S}^0 = \mathbf{T} - \langle \mathbf{m}_A \rangle \mathbf{S}^A$  by means of Eq. (6.4)<sub>2</sub>.

Summarizing the results obtained above, we see that the macro-constitutive (averaged) relations for thermo-elastic/viscoplastic composite materials are given by Eqs. (6.21) where the macro-parameters  $S_{ij}^A$  play a role of the internal variables being governed by the evolution equation (6.19). The above equations have to be considered together with Eqs.(6.16), (6.12) (6.15)<sub>2</sub> and (6.17).

If the material of the r.v.e. is thermo-elastic-plastic, then instead of Eqs. (3.4) we take into account Eqs. (3.5) where the elastic part and inelastic part of the constitutive strain rate tensor are combined together in the elasto-plastic constitutive matrices  $\mathbf{a}^{EP}$ ,  $\mathbf{b}^{EP}$ ; the possible dependence of these matrices on the strain hardening parameters is not specified here but has to be remembered. It is easy to see that Eqs. (6.15)<sub>1,2</sub> can be written now as

$$\dot{\mathbf{S}}^{A} = \overline{\mathbf{B}}^{AB} (\langle \mathbf{m}_{B} \nabla l_{a} \rangle \dot{\mathbf{U}}^{a} + (\langle \mathbf{m}_{B} \rangle - \langle \mathbf{m}_{B} \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle) \dot{\mathbf{E}} + (\langle \mathbf{m}_{B} \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{b}} \rangle - \langle \mathbf{m}_{B} \overline{\mathbf{b}} \rangle) \dot{\boldsymbol{\Theta}} ), \dot{\mathbf{U}}^{a} = \overline{\mathbf{A}}^{ab} \langle \nabla l_{b} \mathbf{m}_{B} \rangle \overline{\mathbf{B}}^{BA} ((\langle \mathbf{m}_{A} \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} - \langle \mathbf{m}_{A} \rangle) \dot{\mathbf{E}} + (\langle \mathbf{m}_{A} \overline{\mathbf{b}} \rangle - \langle \mathbf{m}_{A} \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{b}} \rangle) \dot{\boldsymbol{\Theta}} ,$$

where we have denoted  $\overline{\mathbf{a}} \equiv \mathbf{a}^{EP}$ ,  $\overline{\mathbf{b}} \equiv \mathbf{b}^{EP}$  and where

(6.23) 
$$[\overline{\mathbf{B}}^{AB}]_{6N\times 6N}^{-1} \equiv [\langle \mathbf{m}_A \overline{\mathbf{a}} \mathbf{m}_B \rangle - \langle \mathbf{m}_A \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{a}} \mathbf{m}_B \rangle]_{6N\times 6N},$$
$$[\overline{\mathbf{A}}^{ab}]_{3n\times 3n}^{-1} \equiv [\langle \nabla l_a \mathbf{m}_A \rangle \overline{\mathbf{B}}^{AB} \langle \mathbf{m}_B \nabla l_b \rangle]_{3n\times 3n},$$

under assumption that the above inverses exist. Eliminating  $\dot{U}^a$  from Eqs. (6.22) and denoting

(6.24) 
$$\widehat{\mathbf{B}}^{AB} \equiv \overline{\mathbf{B}}^{AB} - \overline{\mathbf{B}}^{AC} \langle \mathbf{m}_C \nabla l_a \rangle \overline{\mathbf{A}}^{ab} \langle \nabla l_b \mathbf{m}_D \rangle \overline{\mathbf{B}}^{DB} ,$$
$$\overline{\mathbf{D}}^A \equiv \widehat{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \rangle - \langle \mathbf{m}_B \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1}) ,$$
$$\overline{\mathbf{B}}^A \equiv \widehat{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{b}} \rangle - \langle \mathbf{m}_B \overline{\mathbf{b}} \rangle) ,$$

we obtain

(6.25) 
$$\dot{\mathbf{S}}^{A}(\tau) = \overline{\mathbf{D}}^{A}(\mathbf{T}(\tau), \mathbf{S}(\tau), \Theta(\tau), \dot{\mathbf{T}}(\tau), \dot{\mathbf{S}}(\tau))\dot{\mathbf{E}}(\tau) + \overline{\mathbf{B}}^{A}(\mathbf{T}(\tau), \mathbf{S}(\tau), \Theta(\tau), \dot{\mathbf{T}}(\tau), \dot{\mathbf{S}}(\tau))\dot{\Theta}(\tau),$$

where  $S = {S^1(\tau), ..., S^N(\tau)}$ . Combining Eqs. (6.6)<sub>1</sub>, (3.5), (6.1)<sub>3</sub> and (6.4)<sub>2</sub> and setting

(6.26) 
$$\overline{\mathbf{D}} \equiv \langle \overline{\mathbf{a}} \rangle^{-1} + (\langle \mathbf{m}_A \rangle - \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{a}} \mathbf{m}_A \rangle) \widehat{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \rangle - \langle \mathbf{m}_B \overline{\mathbf{a}} \rangle \langle \mathbf{a} \rangle^{-1}) , \\ \overline{\mathbf{B}} \equiv -\langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{b}} \rangle + (\langle \mathbf{m}_A \rangle - \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{a}} \mathbf{m}_A \rangle) \widehat{\mathbf{B}}^{AB} (\langle \mathbf{m}_B \overline{\mathbf{a}} \rangle \langle \overline{\mathbf{a}} \rangle^{-1} \langle \overline{\mathbf{b}} \rangle - \langle \mathbf{m}_B \overline{\mathbf{b}} \rangle) ,$$

we also obtain

(6.27) 
$$\dot{\mathbf{T}}(\tau) = \overline{\mathbf{D}}(\mathbf{T}(\tau), \dot{\mathbf{T}}(\tau), \mathbf{S}(\tau), \dot{\mathbf{S}}(\tau), \Theta(\tau))\dot{\mathbf{E}}(\tau) + \overline{\mathbf{B}}(\mathbf{T}(\tau), \dot{\mathbf{T}}(\tau), \mathbf{S}(\tau), \dot{\mathbf{S}}(\tau), \Theta(\tau))\dot{\Theta}(\tau).$$

The results obtained above represent the macro-constitutive relations for thermoelasto-plastic composite materials, given in the form (6.27) where  $S_{ij}^A(\tau)$  can be treated as internal variables governed by the evolution equation (6.25). The forementioned equations have to be considered together with Eqs.(6.16) and (6.12) where the macro-parameters  $U_i^a(\tau)$  are determined by Eqs. (6.22)<sub>2</sub>.

The macro-constitutive relations for composite materials have to be consistent with the macro-dissipation inequality (6.8). Independently of the macro-constitutive relations, we have derived from the proposed method of the local macro-modelling also the local averaged equations of motion  $(6.4)_1$  and the local averaged equation of the energy balance  $(6.5)_1$ , the form of which is independent of the material structure of r.v.e. The macro-constitutive functions defined by Eqs. (6.18) and (6.20) or Eqs. (6.24) and (6.26) and those in Eqs. (6.16) and (6.12) will be identified with the macro-material properties of the composite structure under consideration. It has to be emphasized that we consider here only a certain mathematical model of the constraints (6.1) and have been obtained under the localization assumption. Let us observe that the constraints (6.1) have a form similar to that used in the finite element method and hence the adaptive procedures can be used.

Now we shall pass to the averaged form of the loading boundary conditions for the composite structure. To this end we introduce the concept of the representative boundary element (r.b.e.) which will be treated, roughly speaking, as a small element of the composite boundary (compared to the whole structure) but large enough to describe the oscillatory character of surface tractions and heat input. The r.b.e. will be analyzed as a smooth part S of a boundary  $\partial W$  of a region W occupied by the composite; for the sake of simplicity we assume that on S both surface tractions  $\hat{t}_i(\mathbf{y}, \tau), \mathbf{y} \in S$  and a heat input  $\hat{\beta}(\mathbf{y}, \tau), \mathbf{y} \in S$ , are known a priori. Moreover, we assume that W is sufficiently small and the macro-modelling procedure can be applied to W. In order to do this, the formulae for  $t_i^L(\mathbf{y}, \tau)$  and  $\beta^L(\mathbf{y}, \tau)$  in the loading relations (6.2) (with V replaced by W) have to be substituted by

$$t_i^L(\mathbf{y},\tau) = (T_{ij}(\tau) + T_{ijk}(\tau)y_k)n_j(\mathbf{y}),$$
  
$$\beta^L(\mathbf{y},\tau) = (H_i(\tau) + H_{ik}(\tau)y_k)n_i(\mathbf{y}) \quad \text{if} \quad \mathbf{y} \in \partial W \setminus \overline{S},$$
  
$$t_i^L(y,\tau) = \hat{t}_i(\mathbf{y},\tau), \quad \beta^L(\mathbf{y},\tau) = \hat{\beta}(\mathbf{y},\tau) \quad \text{if} \quad \mathbf{y} \in S.$$

We also denote

(6.28) 
$$\langle \langle \psi \rangle \rangle = \frac{1}{\operatorname{area}S} \int_{S} \psi(\mathbf{y}) \, da(\mathbf{y})$$

for an arbitrary integrable function  $\psi(\cdot)$ . It can be shown that the macro-modelling procedure described above leads to the averaged relations of thermomechanics in W and to the extra conditions

(6.29) 
$$T_{ij}(\tau)\langle\langle n_j \rangle\rangle = \langle\langle \hat{t}_i \rangle\rangle\langle \tau \rangle, \quad H_i(\tau)\langle\langle n_i \rangle\rangle = \langle\langle \hat{\beta} \rangle\rangle\langle \tau \rangle, \quad \tau \in [\tau_0, \tau_f]$$

which represent the averaged form of the natural boundary conditions for the composite structure.

#### 7. Global macro-modelling

In order to formulate the governing relations for the whole composite structure, we have to make precise the intuitive concepts of the r.v.e. and r.b.e. which were introduced in Sect. 6 without any relation to the composite material structure under consideration. For the sake of simplicity we restrict ourselves to the macroscopically regular structures, i.e., we assume that the macro-properties of the composite do not suffer jump discontinuities.

Let  $\Omega$  be the regular region occupied by the composite body in its referential configuration. Let for every  $\tau \in [\tau_0, \tau_f]$  on the part  $\Gamma, \Gamma \subset \partial \Omega$ , of the boundary the surface tractions  $\hat{t}_i(\cdot, \tau)$  and heat supply  $\hat{\beta}(\cdot, \tau)$  be known and on the remaining part  $\partial \Omega \setminus \overline{\Gamma}$ the displacements  $u_i(\cdot, \tau)$  be prescribed. Let us assign to every  $\mathbf{x} \in \Omega$  and  $\mathbf{z} \in \Gamma$  the non-empty open sets  $V_{\mathbf{x}}$  and  $S_{\mathbf{z}}$ , respectively, such that  $\mathbf{x} \in \overline{V}_{\mathbf{x}} \subset \Omega$ ,  $\mathbf{z} \in \overline{S}_{\mathbf{z}} \subset \Gamma$ . From the purely formal point of view and under the assumption that  $V_{\mathbf{x}}$  and  $S_{\mathbf{z}}$  are sufficiently small (compared to length of dimensions of  $\Omega$  and  $\Gamma$ , respectively), we can substitute  $V_{\mathbf{x}} = V$ and  $S_{\mathbf{z}} = S$  in the macro-modelling procedure proposed in Sect. 6, obtaining the fields of the macro-relations defined on  $\Omega$  and the averaged boundary conditions defined on  $\Gamma$ . The idea of global macro-modelling is based on the physical fact that in many engineering problems there exists a special choice of sets  $V_{\mathbf{x}}$ ,  $\mathbf{x} \in \Omega$ , and  $S_{\mathbf{z}}$ ,  $\mathbf{z} \in \Gamma$ , such that every  $V_{\mathbf{x}}$ ,  $S_{\mathbf{z}}$  can play a role of a certain representative element. To specify such elements, we introduce the following:

GLOBAL MACRO-MODELLING ASSUMPTION. There exist the mappings

(7.1) 
$$\Omega \ni \mathbf{x} \to V_{\mathbf{x}}, \quad \Gamma \ni \mathbf{z} \to S_{\mathbf{z}},$$

such that:

(i) For every  $\mathbf{x} \in \Omega$ ,  $\mathbf{z} \in \Gamma$ , the maximum length dimension  $l_{\mathbf{x}}$  of  $V_{\mathbf{x}}$  and the maximum length dimension  $l_{\mathbf{z}}$  of  $S_{\mathbf{z}}$  are negligibly small as compared to the minimum characteristic length dimensions of  $\Omega$  and  $\Gamma$ , respectively.

(ii) For every  $\mathbf{x} \in \Omega$  and every  $\Delta \mathbf{x} \in \Omega - \mathbf{x}$ ,  $|\Delta \mathbf{x}| < l_{\mathbf{x}}$ , all macro-constitutive functions related to  $V_{\mathbf{x}+\Delta \mathbf{x}}$  can be approximated by the pertinent macro-constitutive functions related to  $V_{\mathbf{x}}$ .

(iii) For every  $z \in \Gamma$  and every  $\Delta z \in \Gamma - z$ ,  $|\Delta z| < l_z$ , the averaged boundary conditions related to  $S_{z+\Delta z}$  can be approximated by the averaged boundary conditions related to  $S_z$ .

Under this assumption every  $V_x$  will be referred to as the r.v.e. of the composite material in the vicinity of x. Similarly, every  $S_z$  will be called the r.b.e. in the vicinity of z. For the periodic material structure all r.v.e. coincide and we pass to the trivial case of the global macro-modelling which is known under the term homogenization.

In the sequel we shall assume that the global macro-modelling assumption holds and hence all macro-entities introduced in Sect. 6 depend on  $\mathbf{x} \in \Omega$  (or on  $\mathbf{z} \in \Gamma$  in Eqs. (6.29)).

From the computational point of view we can also assume that all macro-fields defined on  $\Omega$  and  $\Gamma$  also satisfy the regularity conditions required below; to this end a certain formal regularization of the composite structure may be necessary. Then, for an arbitrary but fixed  $\mathbf{x}, \mathbf{x} \in \Omega$ , and under the localization assumption, the "micro"-coordinates  $\mathbf{y} \in \overline{V}_{\mathbf{x}}$  in Eqs. (6.1) and (6.2) represent the infinitesimal increments (in the sense of the nonstandard analysis, see [8]) of the "macro"-coordinates  $\mathbf{x} \in \Omega$ . In order to interrelate both kinds of coordinates, we have to assume that

(7.2) 
$$F_{ij}(\mathbf{x},\tau) = U_{i,j}(\mathbf{x},\tau), \quad G_i(\mathbf{x},\tau) = \Theta_{,i}(\mathbf{x},\tau), T_{ikk}(\mathbf{x},\tau) = T_{ik,k}(\mathbf{x},\tau), \quad H_{ii}(\mathbf{x},\tau) = H_{i,i}(\mathbf{x},\tau), \quad \mathbf{x} \in \Omega, \quad \tau \in [\tau_0,\tau_f].$$

The above conditions imply the continuity of a passage from an arbitrary (infinitely small) representative volume element to any adjacent element and can be referred to as the macro-compatibility conditions. It has to be emphasized that the form of an arbitrary macro-constitutive function in every  $V_x$ ,  $x \in \Omega$ , from a numerical viewpoint, can be treated as constant but it can be quite different in distant parts of the composite. If such a situation takes place, then the composite structure under consideration will be referred to as macro-inhomogeneous structure.

#### 8. Averaged thermodynamics of composite materials

Summarizing the obtained results, we conclude that the averaged thermodynamics is governed by the following relations:

(i) The equations of motion and energy

(8.1) 
$$T_{ij,j}(\mathbf{x},\tau) + \langle \varrho b_i \rangle (\mathbf{x},\tau) = \langle \varrho \rangle (\mathbf{x}) \ddot{U}_i(\mathbf{x},\tau),$$

$$\langle \varrho \varepsilon \rangle(\mathbf{x}, \tau) = H_{i,i}(\mathbf{x}, \tau) + T_{ij}(\mathbf{x}, \tau) \dot{E}_{ij}(\mathbf{x}, \tau) + \langle \varrho \zeta \rangle(\mathbf{x}, \tau), \quad \mathbf{x} \in \Omega$$

with the averaged boundary conditions

(8.2) 
$$T_{ij}(\mathbf{x},\tau)\langle\langle n_j\rangle\rangle(\mathbf{x}) = \langle\langle \hat{t}_i\rangle\rangle(\mathbf{x},\tau), \quad H_i(\mathbf{x},\tau)\langle\langle n_i\rangle\rangle(\mathbf{x}) = \langle\langle \hat{\beta}\rangle\rangle(\mathbf{x},\tau), \quad \mathbf{x}\in\Gamma,$$

and macro strain - displacement relations

(8.3) 
$$E_{ij}(\mathbf{x},\tau) = U_{(i,j)}(\mathbf{x},\tau), \quad \mathbf{x} \in \Omega$$

(ii) The macro-dissipation inequality

(8.4) 
$$\overline{\langle \varrho \eta^C \rangle}(\mathbf{x},\tau) - \overline{\langle \varrho \varepsilon \rangle} \Theta(\mathbf{x},\tau)^{-1} + S^0_{ij}(\mathbf{x},\tau) \dot{E}_{ij}(\mathbf{x},\tau) \Theta(\mathbf{x},\tau)^{-1} + S^A_{ij}(\mathbf{x},\tau) D_{Aij}(\mathbf{x},\tau) \Theta(\mathbf{x},\tau)^{-1} + H_i(\mathbf{x},\tau) \Theta_{,i}(\mathbf{x},\tau) \Theta(\mathbf{x},\tau)^{-2} \ge 0.$$

(iii) The macro-constitutive relations for a class of inelastic materials under consideration

$$\dot{E}_{ij}(\mathbf{x},\tau) = \langle \hat{d}_{ji} \rangle (\mathbf{x}; \mathbf{S}^0(\mathbf{x},\tau), \mathbf{S}(\mathbf{x},\tau), \dot{\mathbf{S}}^0(\mathbf{x},\tau), \dot{\mathbf{S}}(\mathbf{x},\tau), \boldsymbol{\Theta}(\mathbf{x},\tau), \dot{\boldsymbol{\Theta}}(\mathbf{x},\tau)) ,$$
(8.5)
$$\mathbf{S} \equiv \{\mathbf{S}^1, \dots, \mathbf{S}^N\} ,$$

$$D_{Aij}(\mathbf{x},\tau) = \langle \mathbf{m}_{Aijkl} \widehat{d}_{kl} \rangle (\mathbf{x}; \mathbf{S}^{0}(\mathbf{x},\tau), \mathbf{S}(\mathbf{x},\tau), \dot{\mathbf{S}}^{0}(\mathbf{x},\tau), \dot{\mathbf{S}}(\mathbf{x},\tau), \Theta(\mathbf{x},\tau), \dot{\Theta}(\mathbf{x},\tau));$$

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(8.6) 
$$\langle \varrho \varphi^C \rangle(\mathbf{x}, \tau) = \langle \varrho \varphi^C \rangle(\mathbf{x}, \tau) + \Theta(\mathbf{x}, \tau) \langle \varrho \eta^C \rangle(\mathbf{x}, \tau) ,$$
$$\langle \varrho \varphi^C \rangle(\mathbf{x}, \tau) = \langle \varrho \widehat{\varphi} \rangle(\mathbf{x}; \mathbf{E}(\mathbf{x}, \tau), \mathbf{U}(\mathbf{x}, \tau), \Theta(\mathbf{x}, \tau)) , \quad \mathbf{U} \equiv \{\mathbf{U}^1, \dots, \mathbf{U}^n\} ,$$
$$\langle \varrho \eta^C \rangle(\mathbf{x}, \tau) = \langle \varrho \widehat{\eta} \rangle(\mathbf{x}; \mathbf{E}(\mathbf{x}, \tau), \mathbf{U}(\mathbf{x}, \tau), \Theta(\mathbf{x}, \tau)) ;$$

$$H_{i}(\mathbf{x},\tau) = \langle k_{ij} \rangle(\mathbf{x}) \Theta_{,j}(\mathbf{x},\tau) + \langle k_{ij} l_{a,j} \rangle(\mathbf{x}) G^{a}(\mathbf{x},\tau) ,$$
  
$$0 = \langle k_{ij} l_{a,i} \rangle(\mathbf{x}) \Theta_{,j}(\mathbf{x},\tau) + \langle k_{ij} l_{a,i} l_{b,j} \rangle(\mathbf{x}) G^{b}(\mathbf{x},\tau) , \quad \mathbf{x} \in \Omega .$$

(iv) The extra interrelations between the macro-parameters

$$T_{ij}(\mathbf{x},\tau) = S^0_{ij}(\mathbf{x},\tau) + \langle m_{Aijkl} \rangle(\mathbf{x}) S^A_{kl}(\mathbf{x},\tau) ,$$
  
$$D_{Akl}(\mathbf{x},\tau) = \langle m_{Aklij} \rangle(\mathbf{x}) \dot{E}_{ij}(\mathbf{x},\tau) + \langle m_{Aklij} l_{a,(i)} \rangle(\mathbf{x}) U^a_{ij}(\mathbf{x},\tau) ,$$

$$\langle l_{a,j} m_{Aijkl} \rangle(\mathbf{x}) S^A_{kl}(\mathbf{x}, \tau) = 0, \quad \mathbf{x} \in \Omega.$$

The above equations have to hold for every  $\tau \in [\tau_0, \tau_f]$ . Under the condition that the constraints (6.1) are well posed for the elasto-inelastic materials considered, Eqs. (8.1)–(8.8) represent a certain macroscopically equivalent medium for the inelastic composite medium with highly oscillating material properties. The specifications of the constitutive function  $\widehat{d_{ij}}(\cdot)$ , discussed in Sect. 6, lead to the macro-models of elastic/viscoplastic and elasto-plastic composites, governed by Eqs. (6.19) and (6.21) and Eqs. (6.25) and (6.27), respectively, where all functions also depend on the macro-coordinates  $\mathbf{x} \in \Omega$ . The analysis of special cases of Eqs. (8.1)–(8.8) and certain engineering applications of the proposed averaged thermodynamics as well as various specifications of the constraints (6.1) will be presented in the forthcoming papers.

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