

# Multiscale Constitutive Modelling of the Influence of Anisotropy Effects on Fracture Phenomena in Inelastic Solids

Piotr PERZYNA

*Institute of Fundamental Technological Research*  
*Polish Academy of Sciences*  
Pawińskiego 5B, 02-106 Warszawa, Poland  
e-mail: pperzyna@ippt.pan.pl

The main objective of the present paper is the consistent development of the thermodynamical theory of elasto-viscoplasticity within the framework of a unique constitutive material structure. The focus of attention on the description of the influence of anisotropy effects on fracture phenomena is proposed.

In the first part a general principle of determinism is formulated and a unique constitutive material structure is developed. The original conception of the intrinsic state of a particle  $X$  during motion of a body  $\mathcal{B}$  has been assumed. A notion of the method of preparation of the deformation-temperature configuration of a particle  $X$  has been proposed as a simple way of the gathering information for the description of the internal dissipation. As the basis of the thermodynamical requirements the dissipation principle in the form of the Clausius-Duhem inequality is assumed. By particular assumption of the method of preparation space for a unique constitutive material structure the internal state variable material structure has been constructed. In the second part the thermodynamical theory of elasto-viscoplasticity within the framework of the internal state variable material structure is formulated. Introduction of a finite set of the internal state variables is based on multiscale considerations in analysis of the physical foundations of inelastic solids and experimental observation results. Particular attention is focused on the determination of the evolution laws for the introduced internal state variables. Fracture criterion based on the evolution of the anisotropic intrinsic microdamage is proposed.

## 1. PROLOGUE

A main objective of the present paper is the development of the thermodynamical theory of elasto-viscoplasticity as a unique material constitutive structure within the framework of a general covariant deterministic theory. We would like to focus attention on the description of the influence of anisotropy effects

on fracture phenomena as well as on multiscale considerations in the analysis of the physical foundations and experimental motivations.

By a notion of the thermodynamical theory we understand such, which compatible with the principles of thermodynamical processes describes mechanical and thermal phenomena and their interactions.

A theory is called covariant if it is invariant with respect to arbitrary diffeomorphisms (any motion). A theory is deterministic if its internal structure assures a unique evolution of the intrinsic states and it exists a unique mapping between the intrinsic states and values of reactions (cf. NAGEL [61]).

A good physical theory has to describe large range of phenomena based on several simple postulates and should from it result determined predictions, which has to be investigated and according to that what emphasized Karl Popper (cf. POPPER [104]), in principle be suitable to experimental falsification.

Whenever the result of experimental observations agrees with the theoretical predictions, the tested theory becomes certain that is reliable and our confidence to it is growing up, but if new experimental result disclaims theory we have to quit it or to improve it.

The results of experimental observations fulfil in the development of the physical theory a manifold role. The crux of the matter has been presented by Richard Feynman in his Lectures on Physics [37]: “The principle of science, the definition, almost, is the following: The test of all knowledge is experiment. Experiment is the sole judge of scientific “truth”. But what is the source of knowledge? Where do the laws that are to be tested come from? Experiment, itself, helps to produce these laws, in the sense that it gives us hints. But also needed is imagination to create from these hints the great generalizations – to guess at the wonderful, simple, but very strange patterns beneath them all, and then to experiment to check again whether we have made the right guess”.

Experiment precisely suggests that for proper description of the thermomechanical couplings we have to base our considerations on thermodynamics.

We would like to show advantages, which can be achieved to base the considerations on thermodynamical processes and simultaneously to propose new conception concerning the support the phenomenological thoughts on the results of physics of solids as well as on micro-, meso- and macroscopic, i.e. multiscale experimental investigations. It would be unrealistic to include in the description all the effects observed experimentally. Constitutive modelling is understood as a reasonable choice of effects, which are most important for the explanation of the phenomena described.

Experimental observations concerning investigation of dynamic loading processes have shown that formation of microshear bands influences the evolution of microstructure of material. We can conclude that microshear banding con-

tributes to viscoplastic strain rate effects. On the other hand analysis of recent experimental observations concerning investigations of fracture phenomena under dynamic loading processes suggests that there are two kinds of induced anisotropy: (i) the first caused by the residual type stress produced by the heterogeneous nature of the finite plastic deformation in polycrystalline solids; (ii) the second the fracture induced anisotropy generated by the evolution of the microdamage mechanism. It is noteworthy to stress that both these induced anisotropy effects are coupled.

Section 2 is devoted to the description of kinematics of finite deformation and the stress tensors. The fundamental measures of total deformation are introduced. The description is based on notions of the Riemannian space on manifolds and the tangent space. A multiplicative decomposition of the deformation gradient is adopted. The decomposition of the strain tensor into the elastic and viscoplastic parts is presented. The Lie derivative is used to define all objective rates for the introduced vectors and tensors. The rates of the deformation tensor and the stress tensor are precisely defined.

A general unique constitutive material structure is developed in Sec. 3. The original conception of the intrinsic state of a particle  $X$  during motion of a body  $\mathcal{B}$  has been assumed. A notion of the method of preparation of the deformation-temperature configuration of a particle  $X$  has been proposed as simple way of the gathering information for the description of the internal dissipation. A general principle of determinism for thermodynamical processes has been formulated. The topology for the intrinsic state space and some smoothness assumption for processes and response functions (functionals) are postulated. As the basis of thermodynamic requirements the dissipation principle in the form of the Clausius-Duhem inequality is assumed. The dissipation principle implies two fundamental criteria, namely the criterion of the selection of the response functions (functionals) and the criterion of the accessibility of the intrinsic states. The principle of the increase of entropy has been also deduced. These results have a great importance to the thermodynamical theory of inelastic materials.

In Sec. 4 the internal state variable constitutive structure is presented. Assuming that the method of preparation space for a unique constitutive material structure is a finite dimensional vector space and postulating that the initial value problem for the element of the method of preparation space has unique solutions we construct the material structure with internal state variables. The rate of internal dissipation function for the internal state variable material structure is obtained. From this results we can directly observed that full information given in the method of preparation at the actual intrinsic state essentially determines the rate of internal dissipation for this intrinsic state. This conclusion is of fundamental importance for the physical interpretation of the internal state variables.

Section 5 is focussed on the development of thermo-elasto-viscoplastic constitutive model of a material, which takes into consideration both mentioned earlier induced anisotropy effects as well as observed contribution to strain rate effects generated by microshear banding. The model is developed within the thermodynamic framework of the rate type covariance unique constitutive structure with a finite set of the internal state variables. A set of internal state variables is motivated by experimental observation results, physical foundations and multiscale heuristic considerations, and consists of one scalar and two tensors, namely the equivalent inelastic deformation  $\epsilon^p$ , the second order microdamage tensor  $\boldsymbol{\xi}$ , with the physical interpretation that  $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi$  defines the volume fraction porosity and the residual stress tensor (the back stress)  $\boldsymbol{\alpha}$ .

The equivalent inelastic deformation  $\epsilon^p$  describes the dissipation effects generated by viscoplastic flow phenomena, the microdamage tensor  $\boldsymbol{\xi}$  takes into account the anisotropic intrinsic microdamage mechanisms on internal dissipation and the back stress tensor  $\boldsymbol{\alpha}$  aims at the description of dissipation effects caused by the kinematic hardening. To describe suitably the influence of both induced anisotropy effects and the stress triaxiality observed experimentally the new kinetic equations for the microdamage tensor  $\boldsymbol{\xi}$  and for the back stress tensor  $\boldsymbol{\alpha}$  are proposed.

The relaxation time is used as a regularization parameter. To describe the contribution to strain rate effects generated by microshear banding we propose to introduce certain scalar function which affects the relaxation time  $T_m$  in the viscoplastic flow rule. Fracture criterion based on the evolution of the anisotropic intrinsic microdamage is formulated.

The purpose of the development of this theory is in future applications for the description of important problems in modern manufacturing processes, and particularly for meso-, micro-, and nano-mechanical issues<sup>1)</sup>. This description is needed for the investigation by using the numerical methods how to avoid unexpected plastic strain localization and localized fracture phenomena in new manufacturing technology.

## 2. KINEMATICS OF FINITE DEFORMATION AND FUNDAMENTAL DEFINITIONS

### *2.1. Fundamental measures of total deformation*

Our notation throughout is as follows:  $\mathcal{B}$  and  $\mathcal{S}$  are manifolds, points in  $\mathcal{B}$  are denoted  $\mathbf{X}$  and those in  $\mathcal{S}$  by  $\mathbf{x}$ . The tangent spaces are written  $T_{\mathbf{X}}\mathcal{B}$  and

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<sup>1)</sup>Good examples of such applications are very recent publications as follows: GLEMA *et al.* [44], NOWACKI *et al.* [66] and PERZYNA [93, 94].

$T_{\mathbf{x}}\mathcal{S}$ . Coordinate systems are denoted  $\{X^A\}$  and  $\{x^a\}$  for  $\mathcal{B}$  and  $\mathcal{S}$ , respectively, with corresponding bases  $\mathbf{E}_A$  and  $\mathbf{e}_a$  and dual bases  $\mathbf{E}^A$  and  $\mathbf{e}^a$ .

Let us take the Riemannian spaces on manifolds  $\mathcal{B}$  and  $\mathcal{S}$ , i.e.  $\{\mathcal{B}, \mathbf{G}\}$  and  $\{\mathcal{S}, \mathbf{g}\}$ , the metric tensors  $\mathbf{G}$  and  $\mathbf{g}$  are defined as follows  $\mathbf{G} : T\mathcal{B} \rightarrow T^*\mathcal{B}$  and  $\mathbf{g} : T\mathcal{S} \rightarrow T^*\mathcal{S}$ , where  $T\mathcal{B}$  and  $T\mathcal{S}$  denote the tangent bundles of  $\mathcal{B}$  and  $\mathcal{S}$ , respectively, and  $T^*\mathcal{B}$  and  $T^*\mathcal{S}$  their dual tangent bundles.

Let the metric tensor  $G_{AB}$  be defined by  $G_{AB}(\mathbf{X}) = (\mathbf{E}_A, \mathbf{E}_B)_{\mathbf{X}}$ , and similarly define  $g_{ab}$  by  $g_{ab}(\mathbf{x}) = (\mathbf{e}_a, \mathbf{e}_b)_{\mathbf{x}}$ , where  $(\cdot, \cdot)_{\mathbf{X}}$  and  $(\cdot, \cdot)_{\mathbf{x}}$  denote the standard inner products in  $\mathcal{B}$  and  $\mathcal{S}$ , respectively.

Let

$$(2.1) \quad \mathbf{x} = \phi(\mathbf{X}, t)$$

be regular motion, then  $\phi_t : \mathcal{B} \rightarrow \mathcal{S}$  is a  $C^1$  actual configuration (at time  $t$ ) of  $\mathcal{B}$  in  $\mathcal{S}$ . The tangent of  $\phi$  is denoted  $\mathbf{F}$  and is called the deformation gradient of  $\phi$ ; thus  $\mathbf{F} = T\phi$ . For  $\mathbf{X} \in \mathcal{B}$ , we let  $\mathbf{F}(\mathbf{X})$  denote the restriction of  $\mathbf{F}$  to  $T_{\mathbf{X}}\mathcal{B}$ .

Thus

$$(2.2) \quad \mathbf{F}(\mathbf{X}, t) : T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{x}=\phi(\mathbf{X}, t)}\mathcal{S}$$

is a linear transformation for each  $\mathbf{X} \in \mathcal{B}$  and  $t \in I \subset \mathbb{R}$ . For each  $\mathbf{X} \in \mathcal{B}$  there exists an orthogonal transformation  $\mathbf{R}(\mathbf{X}) : T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{x}}\mathcal{S}$  such that  $\mathbf{F} = \mathbf{R} \cdot \mathbf{U} = \mathbf{V} \cdot \mathbf{R}$ . Notice that  $\mathbf{U}$  and  $\mathbf{V}$  operate within each fixed tangent space. We call  $\mathbf{U}$  and  $\mathbf{V}$  the right and left stretch tensor, respectively. For each  $\mathbf{X} \in \mathcal{B}$ ,  $\mathbf{U}(\mathbf{X}) : T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{X}}\mathcal{B}$  and for each  $\mathbf{x} \in \mathcal{S}$ ,  $\mathbf{V}(\mathbf{x}) : T_{\mathbf{x}}\mathcal{S} \rightarrow T_{\mathbf{x}}\mathcal{S}$ .

The material (or Lagrangian) strain tensor  $\mathbf{E} : T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{X}}\mathcal{B}$  is defined by

$$(2.3) \quad 2\mathbf{E} = \mathbf{C} - \mathbf{I}, \quad (\mathbf{I} \text{ denotes the identity on } T_{\mathbf{X}}\mathcal{B}),$$

where

$$(2.4) \quad \mathbf{C} = \mathbf{F}^T \cdot \mathbf{F} = \mathbf{U}^2 = \mathbf{B}^{-1}.$$

The spatial (or Eulerian) strain tensor  $\mathbf{e} : T_{\mathbf{x}}\mathcal{S} \rightarrow T_{\mathbf{x}}\mathcal{S}$  is defined by

$$(2.5) \quad 2\mathbf{e} = \mathbf{i} - \mathbf{c}, \quad (\mathbf{i} \text{ denotes the identity on } T_{\mathbf{x}}\mathcal{S}),$$

where

$$(2.6) \quad \mathbf{c} = \mathbf{b}^{-1} \quad \text{and} \quad \mathbf{b} = \mathbf{F} \cdot \mathbf{F}^T = \mathbf{V}^2.$$

The various strain tensors can be redefined in terms of pull-back and push-forward operations. For the material strain tensor  $\mathbf{E}$  and the spatial strain tensor  $\mathbf{e}$  we have

$$\begin{aligned}
 \mathbf{E}^b &= \phi^*(\mathbf{e}^b), \\
 E_{AB}(\mathbf{X}) &= e_{ab}(\mathbf{x})F_A^a(\mathbf{X})F_B^b(\mathbf{X}), \\
 \mathbf{e}^b &= \phi_*(\mathbf{E}^b), \\
 e_{ab}(\mathbf{x}) &= E_{AB}(\mathbf{X})(\mathbf{F}(\mathbf{X})^{-1})^A_a(\mathbf{F}(\mathbf{X})^{-1})^B_b,
 \end{aligned}
 \tag{2.7}$$

where the symbol  $\flat$  denotes the index lowering operator.

2.2. Finite elasto-viscoplastic deformation

Motivated by the micromechanics of single crystal plasticity we postulate a local multiplicative decomposition of the form

$$\mathbf{F}(\mathbf{X}, t) = \mathbf{F}^e(\mathbf{X}, t) \cdot \mathbf{F}^p(\mathbf{X}, t),
 \tag{2.8}$$

where  $\mathbf{F}^{e-1}$  is interpreted as the local deformation that releases the stresses from each neighborhood  $\mathcal{N}(\mathbf{x}) \subset \phi(\mathcal{B})$  in the current configuration of the body, cf. Fig. 1.

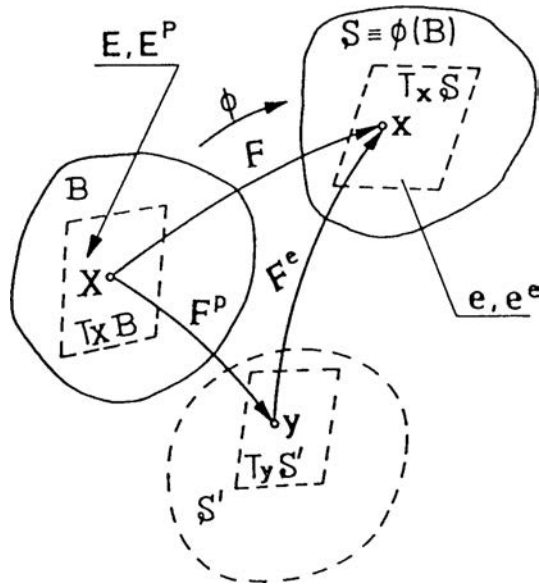


FIG. 1. Schematic representation of the multiplicative decomposition of the deformation gradient.

Let us consider a particle  $X$ , which at time  $t = 0$  occupied the place  $\mathbf{X}$  in the reference (material) configuration  $\mathcal{B}$ , its current place at time  $t$  in the actual

(spatial) configuration  $\mathcal{S}$  is  $\mathbf{x} = \phi(\mathbf{X}, t)$  and its position in the unloaded actual configuration  $\mathcal{S}'$  is denoted by  $\mathbf{y}$ . Thus we have

$$(2.9) \quad \begin{aligned} \mathbf{F}^e &: T_{\mathbf{y}}\mathcal{S}' \rightarrow T_{\mathbf{x}}\mathcal{S}, \\ \mathbf{F}^p &: T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{y}}\mathcal{S}', \end{aligned}$$

where  $T_{\mathbf{y}}\mathcal{S}'$  denotes the tangent space in the unloaded actual configuration  $\mathcal{S}'$ . It is noteworthy that  $\mathbf{F}^e$  and  $\mathbf{F}^p$  defined by (2.9) are linear transformations.

We shall treat the tangent space  $T_{\mathbf{y}}\mathcal{S}'$  as an auxiliary tool which helps to define the plastic strain tensors<sup>2)</sup>.

The plastic strain tensor  $\mathbf{E}^p : T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{X}}\mathcal{B}$  is defined by

$$(2.10) \quad \mathbf{E}^p = \frac{1}{2}(\mathbf{C}^p - \mathbf{I}),$$

where

$$(2.11) \quad \mathbf{C}^p = \mathbf{F}^{pT} \cdot \mathbf{F}^p = \mathbf{U}^{p2} = \mathbf{B}^{p-1} \quad \text{and} \quad \mathbf{E}^e \stackrel{\text{def}}{=} \mathbf{E} - \mathbf{E}^p.$$

Similarly the elastic strain tensor  $\mathbf{e}^e : T_x\mathcal{S} \rightarrow T_x\mathcal{S}$  is defined by

$$(2.12) \quad \mathbf{e}^e = \frac{1}{2}(\mathbf{i} - \mathbf{c}^e),$$

where

$$(2.13) \quad \mathbf{c}^e = \mathbf{b}^{e-1}, \quad \mathbf{b}^e = \mathbf{F}^e \cdot \mathbf{F}^{eT} = \mathbf{V}^{e2} \quad \text{and} \quad \mathbf{e}^p \stackrel{\text{def}}{=} \mathbf{e} - \mathbf{e}^e.$$

It is noteworthy to compare the relation

$$(2.14) \quad \mathbf{F} = \mathbf{R} \cdot \mathbf{U} = \mathbf{V} \cdot \mathbf{R}$$

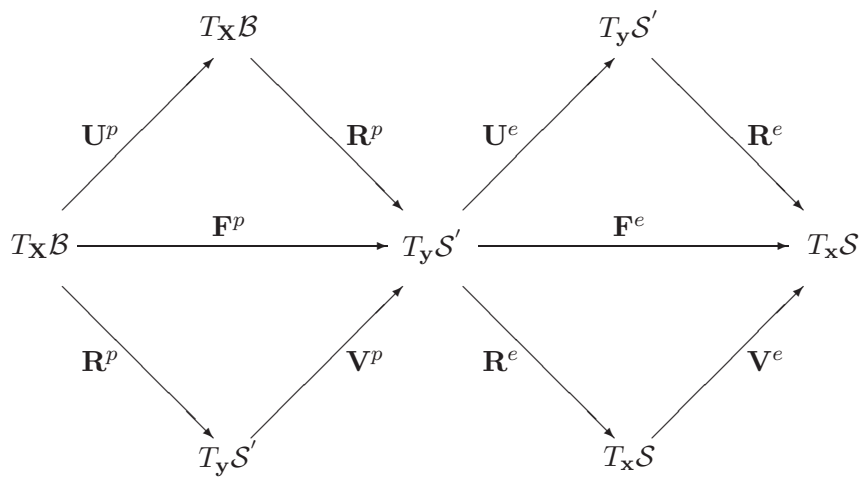
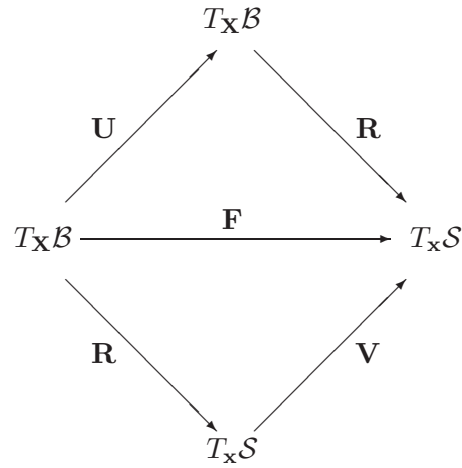
with

$$(2.15) \quad \mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p = \mathbf{R}^e \cdot \mathbf{U}^e \cdot \mathbf{R}^p \cdot \mathbf{U}^p = \mathbf{V}^e \cdot \mathbf{R}^e \cdot \mathbf{V}^p \cdot \mathbf{R}^p.$$

The following commutative diagrams summarize the situation.

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<sup>2)</sup>For precise definition of the finite elasto-plastic deformation see PERZYNA [87] and DUSZEK-PERZYNA, PERZYNA [33]. Different approach to define the finite elasto-plastic deformation has been presented by NEMAT-NASSER [62].



From the second diagram it is clear that the tangent space  $T_y S'$  is playing an auxiliary role indeed.

The plastic tensors  $\mathbf{E}^p$  and  $\mathbf{e}^p$  operate within each fixed tangent space; that is  $\mathbf{E}^p : T_x \mathcal{B} \rightarrow T_x \mathcal{B}$  and  $\mathbf{e}^p : T_x \mathcal{S} \rightarrow T_x \mathcal{S}$ .

We can show that the following relations are valid

$$(2.16) \quad \phi_*(\mathbf{E}^{p^b}) = \mathbf{e}^{p^b}, \quad \phi^*(\mathbf{e}^{e^b}) = \mathbf{E}^{e^b}.$$

### 2.3. Rates of the deformation tensor

Let  $\phi(\mathbf{X}, t)$  be a  $C^2$  motion of  $\mathcal{B}$ . Then the spatial velocity is  $\mathbf{v}_t = \mathbf{V}_t \circ \phi_t^{-1}$ , where  $\mathbf{V}_t = \frac{\partial \phi}{\partial t}$  is the material velocity, i.e.  $\mathbf{v} : \mathcal{S} \times I \rightarrow T\mathcal{S}$ ,  $I \subset \mathbb{R}$ .



The collection of maps  $\phi_{t,s}$  such that for each  $s$  and  $\mathbf{x}$ ,  $t \rightarrow \phi_{t,s}(\mathbf{x})$  is an integral curve of  $\mathbf{v}$ , and  $\phi_{s,s}(\mathbf{x}) = \mathbf{x}$ , is called the flow or evolution operator of  $\mathbf{v}$ , i.e.

$$(2.17) \quad \{\phi_{t,s} \mid \phi_{t,s} = \phi_t \circ \phi_s^{-1} : \phi_s(\mathcal{B}) \rightarrow \phi_t(\mathcal{B})\}$$

and

$$(2.18) \quad \phi_{t,s} \circ \phi_{s,r} = \phi_{t,r}, \quad \phi_{t,t} = \text{identity}$$

for all  $r, s, t \in I \subset \mathbb{R}$ .

If  $\mathbf{t}$  is a  $C^1$  (possible time-dependent) tensor field on  $\mathcal{S}$ , then the Lie derivative of  $\mathbf{t}$  with respect to  $\mathbf{v}$  is defined by<sup>3)</sup>

$$(2.19) \quad L_{\mathbf{v}}\mathbf{t} = \left( \frac{d}{dt} \phi_{t,s}^* \mathbf{t}_t \right) \Big|_{t=s}.$$

If we hold  $t$  fixed in  $\mathbf{t}_t$ , we obtain the autonomous Lie derivative

$$(2.20) \quad \mathcal{L}_{\mathbf{v}}\mathbf{t} = \left( \frac{d}{dt} \phi_{t,s}^* \mathbf{t}_s \right) \Big|_{t=s}.$$

Thus

$$(2.21) \quad L_{\mathbf{v}}\mathbf{t} = \frac{\partial \mathbf{t}}{\partial t} + \mathcal{L}_{\mathbf{v}}\mathbf{t}.$$

If  $\mathbf{t} \in \mathbf{T}^r_s(\mathcal{S})$  (elements of  $\mathbf{T}^r_s(\mathcal{S})$  are called tensors on  $\mathcal{S}$ , contravariant of order  $r$  and covariant of order  $s$ ) then  $L_{\mathbf{v}}\mathbf{t} \in \mathbf{T}^r_s(\mathcal{S})$ .

The spatial velocity gradient  $\mathbf{l}$  is defined by

$$(2.22) \quad \mathbf{l} = D\mathbf{v} : T_{\mathbf{x}}\mathcal{S} \rightarrow T_{\mathbf{x}}\mathcal{S}, \quad \text{i.e.} \quad l_b^a = v^a \Big|_b = \frac{\partial v^a}{\partial x^b} + \gamma_{bc}^a v^c,$$

where  $\gamma_{bc}^a$  denotes the Christoffel symbol for  $\mathbf{g}$ .

The spatial velocity gradient  $\mathbf{l}$  can be expressed as follows

$$(2.23) \quad \begin{aligned} \mathbf{l} = D\mathbf{v} &= \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} = \dot{\mathbf{F}}^e \cdot \mathbf{F}^{e-1} + \mathbf{F}^e \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1}) \cdot \mathbf{F}^{e-1} \\ &= \mathbf{l}^e + \mathbf{l}^p = \mathbf{d} + \boldsymbol{\omega} \mathbf{d}^e + \boldsymbol{\omega}^e + \mathbf{d}^p + \boldsymbol{\omega}^p, \end{aligned}$$

where  $\mathbf{d}$  denotes the spatial rate of deformation tensor and  $\boldsymbol{\omega}$  is called the spin.

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<sup>3)</sup>The algebraic and dynamic interpretations of the Lie derivative have been presented by ABRAHAM *et al.* [2], cf. also MARSDEN, HUGHES [58].

Let us define the material (or Lagrangian) rate of deformation tensor  $\mathbf{D}$  as follows

$$(2.24) \quad \mathbf{D}(\mathbf{X}, t) = \frac{\partial}{\partial t} \mathbf{E}(\mathbf{X}, t).$$

We have very important relation

$$(2.25) \quad \mathbf{d}^b = \mathbf{L}\mathbf{v}\mathbf{e}^b = \phi_* \frac{\partial}{\partial t} (\phi^* \mathbf{e}^b) = \phi_* \left( \frac{\partial}{\partial t} \mathbf{E}^b \right) = \phi_*(\mathbf{D}^b).$$

On the other hand

$$(2.26) \quad \begin{aligned} \mathbf{d}^b = \mathbf{L}\mathbf{v}\mathbf{e}^b &= \mathbf{L}\mathbf{v} \left[ \frac{1}{2} (\mathbf{g} - \mathbf{b}^{-1}) \right]^b = \frac{1}{2} \mathbf{L}\mathbf{v}\mathbf{g} \\ &= \frac{1}{2} (g_{cb} v^c |_a + g_{ac} v^c |_b) \mathbf{e}^a \otimes \mathbf{e}^b, \end{aligned}$$

i.e. the symmetric part of the velocity gradient  $\mathbf{l}$  (the symbol  $\otimes$  denotes the tensor product).

The components of the spin  $\boldsymbol{\omega}$  are given by

$$(2.27) \quad \omega_{ab} = \frac{1}{2} (g_{ac} v^c |_b - g_{cb} v^c |_a) = \frac{1}{2} \left( \frac{\partial v_a}{\partial x^b} - \frac{\partial v_b}{\partial x^a} \right),$$

and

$$(2.28) \quad \mathbf{d}^{e^b} = \mathbf{L}\mathbf{v}\mathbf{e}^{e^b}, \quad \mathbf{d}^{p^b} = \mathbf{L}\mathbf{v}\mathbf{e}^{p^b}.$$

#### 2.4. Rates of the stress tensors

The first Piola-Kirchhoff stress tensor  $P^{aA}$  is the two-point tensor obtained by performing a Piola transformation on the second index of the Cauchy stress tensor  $\boldsymbol{\sigma}$ , i.e.

$$(2.29) \quad P^{aA} = J(\mathbf{F}^{-1})_b^A \sigma^{ab},$$

where  $J$  denotes the Jacobian of the deformation.

The second Piola-Kirchhoff stress tensor  $\mathbf{S}$  is defined as follows

$$(2.30) \quad S^{AB} = (\mathbf{F}^{-1})_a^A P^{aB} = J(\mathbf{F}^{-1})_a^A (\mathbf{F}^{-1})_b^B \sigma^{ab} = (\mathbf{F}^{-1})_a^A (\mathbf{F}^{-1})_b^B \tau^{ab},$$

i.e.

$$(2.31) \quad \mathbf{S} = \phi^*(\boldsymbol{\tau}),$$

where  $\boldsymbol{\tau} = J\boldsymbol{\sigma}$  is called the Kirchhoff stress tensor.

The rate of the Kirchhoff stress tensor  $\boldsymbol{\tau}$  is given by

$$(2.32) \quad \mathbf{L}_v \boldsymbol{\tau} = \phi_* \frac{\partial}{\partial t} (\phi^* \boldsymbol{\tau}) = \phi_* \left( \frac{\partial}{\partial t} \mathbf{S} \right) = \mathbf{F} \cdot \left( \frac{\partial}{\partial t} \mathbf{S} \right) \cdot \mathbf{F}^T \circ \phi_t^{-1}.$$

Let us define

$$(2.33) \quad \begin{aligned} \boldsymbol{\tau}_1 &= \tau^{ab} \mathbf{e}_a \otimes \mathbf{e}_b \in \mathbf{T}^2_0(\mathcal{S}), \\ \boldsymbol{\tau}_2 &= \tau_a{}^b \mathbf{e}^a \otimes \mathbf{e}_b \in \mathbf{T}^1_1(\mathcal{S}), \\ \boldsymbol{\tau}_3 &= \tau^a{}_b \mathbf{e}_a \otimes \mathbf{e}^b \in \mathbf{T}^1_1(\mathcal{S}). \end{aligned}$$

Then

$$(2.34) \quad (\mathbf{L}_v \boldsymbol{\tau}_1)^{ab} = \frac{\partial \tau^{ab}}{\partial t} + \frac{\partial \tau^{ab}}{\partial x^c} v^c - \tau^{cb} \frac{\partial v^a}{\partial x^c} - \tau^{ac} \frac{\partial v^b}{\partial x^c}.$$

is the rate associated with the name OLDROYD (cf. [68]). The Zaremba-Jaumann rate (cf. ZAREMBA [118, 119] and JAUMANN [46]) is defined as follows

$$(2.35) \quad \frac{1}{2} \left[ (\mathbf{L}_v \boldsymbol{\tau}_3)^a{}_c g^{cb} + g^{ac} (\mathbf{L}_v \boldsymbol{\tau}_2)_c{}^b \right] = \frac{\partial \tau^{ab}}{\partial t} + \frac{\partial \tau^{ab}}{\partial x^c} v^c + \tau^{ad} \omega_d{}^b - \tau^{db} \omega_d{}^a.$$

2.5. Fundamental properties of the Lie derivatives

Let us take again  $\mathbf{t} \in \mathbf{T}^r_s(\mathcal{S})$  a given time dependent spatial tensor field on  $\mathcal{S}$  and let  $\zeta$  be a diffeomorphism of  $\mathcal{S}$  to another manifold  $\zeta(\phi(\mathcal{B}))$ , cf. Fig. 2.

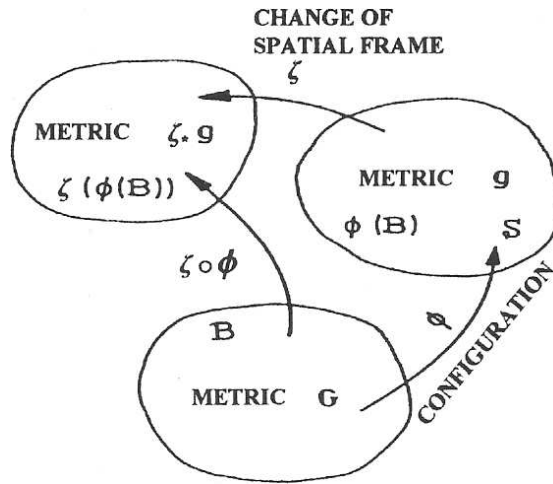


FIG. 2. Schematic representation of the change of spatial frame generated by superposed spatial diffeomorphism.

Any spatial tensor field  $\mathbf{t} \in \mathbf{T}^r_s(\mathcal{S})$  is said to transform objectively under superposed diffeomorphism  $\zeta$  if it transforms according to the rule

$$(2.36) \quad \mathbf{t}' = \zeta_* \mathbf{t},$$

where  $\zeta_*$  is the push-forward operation.

Let  $\mathbf{v}'$  be the velocity field of  $\zeta_t \circ \phi_t$ . Then we have (cf. MARSDEN, HUGHES [58])

$$(2.37) \quad L_{\mathbf{v}'} \mathbf{t}' = \zeta_*(L_{\mathbf{v}} \mathbf{t}).$$

This means that objective tensors have objective Lie derivatives. It is noteworthy to recall here that rates which are objective with respect to diffeomorphism are called covariant.

The Oldroyd rate of the Kirchhoff stress tensor (2.34) is objective with respect to diffeomorphisms while the Zaremba-Jaumann rate (2.35) is objective with respect to isometries. The reason of it is caused by the fact that the operations of raising and lowering indices do not commute with Lie differentiation. This corollary has very important consequences for the formulation of the objective constitutive structures.

If  $f$  is the time dependent scalar field, then the material derivative

$$(2.38) \quad \dot{f} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x^\alpha} v^\alpha.$$

### 3. GENERAL PRINCIPLE OF DETERMINISM. A UNIQUE CONSTITUTIVE MATERIAL STRUCTURE

#### 3.1. Local thermodynamical process

The main objective of this chapter is the development of a unique constitutive material structure. In other words we would like to describe the physical properties of a material of a body  $\mathcal{B}$ . Thus, we shall deal with the thermodynamics of continuous media.

Let us introduce additional denotations in the actual (spatial) configuration  $\phi(\mathcal{B})$  for a body  $\mathcal{B}$  for absolute temperature  $\vartheta(\mathbf{x}, t)$ , the free energy  $\psi(\mathbf{x}, t)$ , the specific (per unit mass) entropy  $\eta(\mathbf{x}, t)$ , the mass density  $\rho(\mathbf{x}, t)$  and the heat flux vector field  $\mathbf{q}(\mathbf{x}, t)$ .

Let us define a local thermodynamical process for a body  $\mathcal{B}$  by using fields determined in the spatial configuration  $\phi_t(\mathcal{B})$  for  $t \in [t_o, t_f]$ .

**Definition 1.** A set of the fields

$$(3.1) \quad \mathcal{P}_{\phi_t(\mathcal{B})} = \{\phi, \vartheta, \rho, \psi, \eta, \boldsymbol{\tau}, \mathbf{q}\}(\mathbf{x}, t)$$

given for every  $\mathbf{x} \in \phi_t(\mathcal{B})$ , for  $t \in [t_o, t_f]$  and satisfying the principles:

(i) conservation of mass

$$(3.2) \quad \dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0;$$

(ii) balance of momentum

$$(3.3) \quad \rho \dot{\mathbf{v}} = \operatorname{div} \left( \frac{1}{J} \boldsymbol{\tau} \right);$$

(iii) balance of angular momentum

$$(3.4) \quad \boldsymbol{\tau} = \boldsymbol{\tau}^T;$$

(iv) balance of energy

$$(3.5) \quad \rho \left( \dot{\psi} + \vartheta \dot{\eta} + \eta \dot{\vartheta} \right) + \operatorname{div} \mathbf{q} = \frac{\rho}{\rho_{\text{ref}}} \boldsymbol{\tau} : \mathbf{d};$$

(v) entropy production inequality

$$(3.6) \quad \frac{1}{\rho_{\text{ref}}} \boldsymbol{\tau} : \mathbf{d} - \left( \eta \dot{\vartheta} + \dot{\psi} \right) - \frac{1}{\rho \vartheta} \mathbf{q} \cdot \operatorname{grad} \vartheta \geq 0;$$

will be called a local thermodynamical process.

In a class of processes for a body  $\mathcal{B}$  we shall favour the processes which satisfied the principles of thermodynamics.

The principle of balance of energy (3.5) expresses the first law of thermodynamics and gives restrictions on the phenomena and the interactions, which we can describe. This principle suggests that our aim of the description will be in mechanical and thermal phenomena.

The different nature represents the entropy production inequality (3.6) called also the reduced dissipation inequality. MARS DEN and HUGHES [58] proved that the reduced dissipation inequality (3.6) is equivalent to the entropy production inequality first introduced by COLEMAN and NOLL [19] in the form of the Clausius-Duhem inequality. In fact the Clausius-Duhem inequality gives a statement of the second law of thermodynamics within the framework of mechanics of continuous media. The entropy production inequality poses some restrictions on the constitutive functions of the response of a material of a body  $\mathcal{B}$ . We can state that the second law of thermodynamics favours in a class of materials the real material. It is noteworthy to cite here Max PLANCK [103], who the problem of thermodynamical restrictions for physical processes understood in very precise way:

“The principle of balance of energy imposes the restrictions on nature processes, since it states, that energy does never appear or does vanish, but it may be only subject to change.

The second law of thermodynamics increases this restriction, since it says that not all kinds of change are possible, but only some of them and under certain determined conditions.”

To relate this thought of Planck to the considered situation we can state that exactly the determination of the restrictions in the description of a material, which satisfy, the realization of the real processes compatible with the principles of thermodynamics is a main problem of the thermodynamical theory of materials.

**Definitions 2.** A local thermodynamical process  $\mathcal{P}_{\phi_t(\mathcal{B})}$  we shall call an admissible process, if it satisfies the constitutive equations for a material in a body  $\mathcal{B}$ .

We assume as the fundamental principle of physics the objectivity of properties of a material, i.e. we postulate that the constitutive equations describing the material in a body  $\mathcal{B}$  have to be invariant with respect to arbitrary diffeomorphism  $\zeta : \mathcal{S} \rightarrow \mathcal{S}$  (any motion).

**Definition 3.** Two local thermodynamical processes

$$(3.7) \quad \{\phi, \vartheta, \rho, \psi, \eta, \boldsymbol{\tau}, \mathbf{q}\} \quad \text{and} \quad \{\phi', \vartheta', \rho', \psi', \eta', \boldsymbol{\tau}', \mathbf{q}'\}$$

related to each other by arbitrary diffeomorphisms (any motion) we shall call isomorphic processes.

**Principle of objectivity of a material** (spatial covariance) may be formulated as follows: If the constitutive equations are satisfied for a local thermodynamical process  $\{\phi, \vartheta, \rho, \psi, \eta, \boldsymbol{\tau}, \mathbf{q}\}$  then they are also satisfied for the isomorphic process  $\{\phi', \vartheta', \rho', \psi', \eta', \boldsymbol{\tau}', \mathbf{q}'\}$ .

**Definition 4.** The four values

$$(3.8) \quad g = (\mathbf{e}, \mathbf{F}, \vartheta, \text{grad } \vartheta)(\mathbf{x}, t)$$

computed for a particle X in actual (spatial) configuration of a body  $\mathcal{B}$  at the instant of time  $t \in [0, d_p]$  we shall call the local deformation-temperature configuration of X at time t.

A set of all possible spatial configurations of a particle X we denote by  $\mathcal{G}$  and shall it call the deformation-temperature configuration space.

**Definition 5.** The four values

$$(3.9) \quad s = (\psi, \eta, \boldsymbol{\tau}, \mathbf{q})(\mathbf{x}, t)$$

given in a particle X at time  $t \in [0, d_Z]$  we shall call the actual local response of a particle X.

A set of all possible responses of a particle X we denote by  $\mathfrak{S}$  and shall call the response space.

Let us consider processes in the configuration space  $\mathcal{G}$  and in the response space  $\mathfrak{S}$ .

A process<sup>4)</sup>

$$(3.10) \quad P = (\mathbf{e}, \mathbf{F}, \vartheta, \text{grad } \vartheta) : [0, d_P] \rightarrow \mathcal{G}$$

will determine the change of the deformation-temperature configuration of a particle X in the interval of time  $[0, d_P]$ . A number  $d_P$  will be called the duration of the process  $P$ , and  $P^i = P(0)$  and  $P^f = P(d_P)$  the initial and final values of the process  $P$ , respectively.

A process

$$(3.11) \quad Z \equiv (\psi, \eta, \boldsymbol{\tau}, \mathbf{q}) : [0, d_Z] \rightarrow \mathfrak{S}$$

will determine the change of the response of a particle X in the interval of time  $[0, d_Z]$ , i.e., the change of the free energy, the entropy, the Kirchhoff stress, and the heat flux.

Let us denote by

$$(3.12) \quad \Pi \equiv \{P | P : [0, d_P] \rightarrow \mathcal{G}\}$$

a set of all deformation-temperature configuration processes, and by

$$(3.13) \quad \mathcal{Z} \equiv \{Z | Z : [0, d_Z] \rightarrow \mathfrak{S}\}$$

a set of all response processes for a particle X.

**Definition 6.** Every pair  $(P, Z) \in \Pi \times \mathcal{Z}$  such that  $\text{Dom } P = \text{Dom } Z$  and for every instant of time  $t \in [0, d_P]$  the dissipation principle in the form of Clausius-Duhem inequality (3.6) is satisfied; will be called a local thermodynamical process.

A set of all thermodynamical processes will be denoted by  $\mathcal{P}_X$ .

### 3.2. Method of preparation

In a set of local thermodynamical processes  $\mathcal{P}_X$  we shall consider a subset which will be compatible with the internal constitutive assumptions describing the intrinsic physical constitution of a body  $\mathcal{B}$ , i.e. compatible with a material<sup>5)</sup>

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<sup>4)</sup>For a thorough discussion of properties of a process and for the definition of a segment of the given process  $P$  and the continuation of the process  $P_1$  with  $P_2$ , see NOLL [64].

<sup>5)</sup>A material as defined by NOLL [64] is an equivalence class of material structures, the equivalence being material isomorphy, cf. also PERZYNA [78].

of a body  $\mathcal{B}$ . Such a subset of a local thermodynamical process space will be called admissible for the constitutive assumptions in question. In a set  $\mathcal{P}_X$  we shall be interested such local thermodynamical processes which have the characteristic property that deformation-temperature processes  $\mathcal{P}$  are in some relation with appropriate response process  $Z$ . Thus, in a set  $\mathcal{P}_X$  we distinguish some subset  $R$ .

**Definition 7.** A subset  $R$  of a set of local thermodynamical processes  $\mathcal{P}_X$  of a particle  $X$  we shall call the constitutive relation, provided that the conditions are satisfied as follows:

- (i)  $\text{pr}_\Pi(R) = \Pi$ ,
- (ii) if  $(P, Z) \in R$  then  $(P_{[0,t]}, Z_{[0,t]}) \in R$  for  $t \in \text{Dom}P$ .

Appearing the relation  $R$  in a set of thermodynamical processes  $\mathcal{P}_X$  causes that locally in the particle  $X$  we introduce the material structure.

**Definition 8.** A system  $(\mathcal{G}, \Pi, R)$  we shall call the body element with the material structure.

The relation  $R$  given in a set of thermodynamical processes  $\mathcal{P}_X$  does not have to be generally right-hand unique, i.e. in general it does not satisfy the condition

$$(3.14) \quad \bigwedge_{P \in \Pi} \bigwedge_{Z_1, Z_2 \in \mathcal{Z}} [(P, Z_1) \in R \wedge (P, Z_2) \in R] \Rightarrow Z_1 = Z_2.$$

If the relation  $R$  has this property, i.e. has been the functional relation, then every process  $P \in \Pi$  corresponds only one (uniquely determined) response process  $Z \in \mathcal{Z}$ .

If this case happens, then the material structure of the element  $(\mathcal{G}, \Pi, R)$  has to be the elastic material structure.

In the case of inelastic dissipative materials the relation  $R$  does not be the functional relation.

From previous consideration follows that if we wish to have the unique relation  $R$  in a set of thermodynamical processes  $\mathcal{P}_X$ , we should to complete our informations about a particle  $X$ . Let us focus our attention on the initial configuration  $P^i = P(0) = g_0$  of a particle  $X$ , from which the deformation-temperature configuration process  $P : [0, d_P] \rightarrow \mathcal{G}$  has been begun. For an elastic material the knowledge of the configuration  $g_0$  determines uniquely the response of a material at instant of time  $t = 0$ , i.e.  $s_0 = (\psi(0), \eta(0), \boldsymbol{\tau}(0), \mathbf{g}(0))$  at a particle  $X$ . In the case of inelastic (dissipative) materials very crucial is also the knowledge in what way the configuration  $g_0$  has been achieved. It is required the additional information about a particle  $X$  in instant of time  $t = 0$ , which is in the configuration  $g_0$ .



A main objective the thermodynamics of inelastic continuous media is to predict the response of a particle X of a body  $\mathcal{B}$ , of which physical properties are know, at the end of a deformation-temperature process. We can give an answer to this question if, and only if, we have full information about particle X before the test, i.e. before a deformation-temperature configuration process. If we have a deformation-temperature configuration process  $P \in \Pi$ , then the definition of the additional information about the initial configuration  $g_0$  of a particle X, which provides for unique determination of the response process  $Z \in \mathcal{Z}_P$  in the response space  $\mathcal{S}$ , being in the relation  $R$  with the process  $P$ , we shall call **the method of preparation**<sup>6)</sup>. In other words the method of preparation should give the additional information to define uniquely the intrinsic state of a particle X of a body  $\mathcal{B}$  during the local thermodynamical process  $P_{\phi_t(B)} \in \mathcal{P}_X$ .

By the intrinsic state of a particle X we define a pair: the transient configuration of a particle X and corresponded it the method of preparation.

It will be shown that a method of preparation of the deformation-temperature configuration of a particle X is needed to describe the internal dissipation of a material. This is a very important feature of the notion of the method of preparation.

To discuss the general relation between processes  $P \in \Pi$  and  $Z \in \mathcal{Z}$  which defines a material structure of a body  $\mathcal{B}$  let us introduce a space  $\mathcal{M}$  connected with the configuration space  $\mathcal{G}$  in such a way that elements of the space  $\mathcal{M}$ , which will be denoted by  $m \in \mathcal{M}$ , are the method of preparation of the corresponding configuration  $g \in \mathcal{G}$ . The space  $\mathcal{M}$  will be called **the method of preparation space**.

**Definition 9.** A non-empty set  $\mathcal{M}$  will be called the method of preparation space for a particle X if

$$(3.15) \quad \bigvee_{\Sigma \subset \mathcal{G} \times \mathcal{M}} \bigvee_{\mathfrak{R}: (\Sigma \times \Pi)^* \rightarrow \mathcal{Z}} \bigwedge_{g \in \mathcal{G}} \bigwedge_{P \in \Pi_g} \bigwedge_{\mathcal{M}_g \subset \mathcal{M}} \mathfrak{R}(g, \cdot, P) : \mathcal{M}_g \rightarrow \mathcal{Z}_P \quad \text{is bijection,}$$

where

$$(3.16) \quad (\Sigma \times \Pi)^* \equiv \left\{ (\sigma, P) \in \Sigma \times \Pi \mid \bigvee_{\mathcal{M}_{P^i} \subset \mathcal{M}} \sigma \in \{P^i\} \times \mathcal{M}_{P^i} \right\},$$

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<sup>6)</sup>For a notion of the method of preparation see BRIDGMAN [9] and GILES [39], cf. also PERZYNA [72, 73, 75, 76] and PERZYNA, KOSIŃSKI [96]. The precise definition of the method of preparation space for a pure mechanical process was first given by PERZYNA, KOSIŃSKI [96]. The generalization to the thermodynamical processes was presented by PERZYNA [77]

denotes a set of pairs the intrinsic state and the deformation-temperature configuration processes  $(\sigma, P)$  such, that the process  $P$  is initiated at the state  $\sigma$ , i.e.  $P^i = g$  if  $\sigma = (g, m)$ ,

$$(3.17) \quad \Pi_g \equiv \{P \in \Pi | P^i = g\}$$

denotes a set of all deformation-temperature configuration processes which are initiated at the configuration  $g \in \mathcal{G}$ , and  $\mathcal{Z}_P$  is a subset of  $\mathcal{Z}$  corresponding to the process  $P$ .

**Definition 10.** A set

$$(3.18) \quad \Sigma \equiv \bigcup_{g \in \mathcal{G}} \{g\} \times \mathcal{M}_g, \quad \mathcal{M}_g \subset \mathcal{M}$$

(constructed by the Definition 9) is called the intrinsic state space<sup>7)</sup> of a particle  $X$  of the element body with the material structure  $(\mathcal{G}, \Pi, R)$ .

The element  $\sigma \in \Sigma$  is a pair of the deformation-temperature configuration and the method of preparation, i.e.

$$(3.19) \quad \sigma \equiv (P(t), M(t)) = (g, m), \quad g \in \mathcal{G}, \quad m \in \mathcal{M}_g,$$

where by  $M$  we denote a process in the method of preparation space  $\mathcal{M}$ , i.e.,  $M : [0, d_P] \rightarrow \mathcal{M}$ .

We define two mappings as follows<sup>8)</sup>

$$(3.20) \quad \widehat{\mathbf{G}} \equiv \text{pr}_{\mathcal{G}} : \Sigma \rightarrow \mathcal{G}, \quad \widehat{\mathbf{M}} \equiv \text{pr}_{\mathcal{M}} : \Sigma \rightarrow \mathcal{M},$$

which determine the projections from the intrinsic space  $\Sigma$  on the configuration space  $\mathcal{G}$  and on the method of preparation space  $\mathcal{M}$ , respectively.

### 3.3. General principle of determinism. Unique material structure

The notion of a method of preparation is connected with a general principle of determinism in mechanics of continuum medium. The principle of determinism

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<sup>7)</sup>The intrinsic state space  $\Sigma$  has been defined by PERZYNA, KOSIŃSKI [96]. It plays a similar role in the theory of materials as the state space introduced by NOLL [64]. The difference between these two notions of state is in the conception of the method of preparation. The elements of the intrinsic state space are pairs. Every pair consists of the local configuration and its method of preparation. There is no notion of the method of preparation in Noll's conception of state. The idea of splitting every element of the intrinsic state space into the local configuration and its method of preparation allows us to characterize precisely the intrinsic state of a particle  $X$  and is of great importance for the development of thermodynamics of dissipative material structures.

<sup>8)</sup>The mappings  $\widehat{\mathbf{G}}$  and  $\widehat{\mathbf{M}}$  were first introduced for a purely mechanical case, the former by NOLL [64] and the latter by PERZYNA, KOSIŃSKI [96].

can be stated as follows: Between an initial deformation-temperature configuration, its method of preparation, a deformation-temperature process beginning at this configuration and a response process of a particle X, there exists a functional relationship. This functional relation will describe a unique material structure in a particle X of a body  $\mathcal{B}$ .

Let us assume that for the body element with the material structure  $(\mathcal{G}, \Pi, R)$  exists the method of preparation space  $\mathcal{M}$ .

According to Definition 9 there exists a mapping

$$(3.21) \quad \mathfrak{R} : (\Sigma \times \Pi)^* \rightarrow \mathcal{Z}.$$

**Definition 11.** The mapping  $\mathfrak{R}$  defined by (3.21) is called the constitutive mapping for the body element with the material structure  $(\mathcal{G}, \Pi, R)$ .

The constitutive mapping  $\mathfrak{R} : (\Sigma \times \Pi)^* \rightarrow \mathcal{Z}$  has the property as follows

$$(3.22) \quad \bigwedge_{\substack{\sigma_1, \sigma_2 \in \Sigma \\ \widehat{\mathbf{G}}(\sigma_1) = \widehat{\mathbf{G}}(\sigma_2)}} \bigwedge_{P \in \Pi_g} \{(\sigma_i, P) \in (\Sigma \times \Pi)^*, \\ i = 1, 2 \wedge \mathfrak{R}(\sigma_1, P) = \mathfrak{R}(\sigma_2, P)\} \Rightarrow \widehat{\mathbf{M}}(\sigma_1) = \widehat{\mathbf{M}}(\sigma_2).$$

**Definition 12.** The system  $(\mathcal{G}, \Pi, \Sigma, \mathfrak{R})$  is called a unique material structure in a particle X of a body  $\mathcal{B}$ .

The constitutive mapping  $\mathfrak{R}$  with the property (3.22) expresses a general principle of determinism of dissipative continuum body.

**A general principle of determinism:** A unique response process  $Z \in \mathcal{Z}$  corresponds to every deformation-temperature process  $P \in \Pi$  beginning at the given intrinsic state  $\sigma \in \Sigma$ .

This statement of a principle of determinism is very general. It concerns thermodynamic processes and is valid for the arbitrary method of preparation space introduced.

A theory can be called deterministic if the analysis of its internal structure shows that from a theoretical description of the intrinsic state of a particle X of a body  $\mathcal{B}$  in an arbitrary initial instant of time results a unique description of the intrinsic state of this particle in the later instant of time and every intrinsic state of particle X corresponds the unique value of the response. In other words, we shall call a theory deterministic if its internal structure assures the unique evolution of the intrinsic states and there exists a unique mapping between the intrinsic states and the values of the responses.

In the definition of the deterministic theory it is included a nature of the irreversibility of the process. The irreversibility results from the turn of the axis of

time. We speak about the initial instant of time and the later instant of time but not about two arbitrary instants of time (cf. GILES [39] and LANDSBERG [53]).

We shall show that the constitutive mapping  $\mathfrak{R}$  generates the evolution function  $\widehat{\mathbf{e}}$  and the material function  $\widehat{\mathbf{S}}$ , which the first assures the evolution of the intrinsic states, and the second guarantees a unique mapping between the intrinsic states and the values of responses.

### 3.4. Evolution of intrinsic states

Let us assume that a unique material structure  $(\mathcal{G}, \Pi, \Sigma, \mathfrak{R})$  is given. If we have the initial intrinsic state and the deformation-temperature process beginning at this intrinsic state we are interested then in the intrinsic state at the end of the process. The problem will be solved if a mapping between the intrinsic state at the end of the deformation-temperature process and the initial intrinsic state is given.

**Definition 13.** It is said that a mapping

$$(3.23) \quad \widehat{\mathbf{e}} : (\Sigma \times \Pi)^* \rightarrow \Sigma$$

is the evolution function, if for every pair  $(\sigma, P) \in (\Sigma \times \Pi)^*$  the equation

$$(3.24) \quad \mathfrak{R}(\widehat{\mathbf{e}}(\sigma, P), P_{(0)}^f) = [\mathfrak{R}(\sigma, P)]^f$$

is satisfied, where  $[\mathfrak{R}(\sigma, P)]^f$  denotes the final value of the response process  $Z = \mathfrak{R}(\sigma, P)$  and  $P_{(0)}^f$  is the deformation-temperature process of duration zero.

### 3.5. The mapping from the intrinsic state space into the response space

In the practical applications it will be convenient to have a mapping from the intrinsic state space  $\Sigma$  into the response space  $\mathfrak{S}$ . So, it is useful to define a new mapping

$$(3.25) \quad \widehat{\mathbf{S}} : \Sigma \rightarrow \mathfrak{S}$$

by the expression

$$(3.26) \quad \widehat{\mathbf{S}}(\sigma) \equiv \mathfrak{R}(\sigma, \widehat{\mathbf{G}}(\sigma)_{(0)}).$$

Taking into account the last expression we can write the definition of the evolution function in the form as follows

$$(3.27) \quad \bigwedge_{t \in \text{Dom} P} \widehat{\mathbf{S}}(\widehat{\mathbf{e}}(\sigma_0, P_{[0,t]})) = [\mathfrak{R}(\sigma_0, P_{[0,t]})]^f.$$

The principle of determinism can be expressed by the relation<sup>9)</sup>

$$(3.28) \quad Z(t) = s = \hat{S}(\hat{\mathbf{e}}(\sigma_0, P)) = \hat{\mathbf{S}}(\sigma)$$

for every  $(\sigma_0, P) \in (\Sigma \times \Pi)^*$ , cf. Fig. 3.

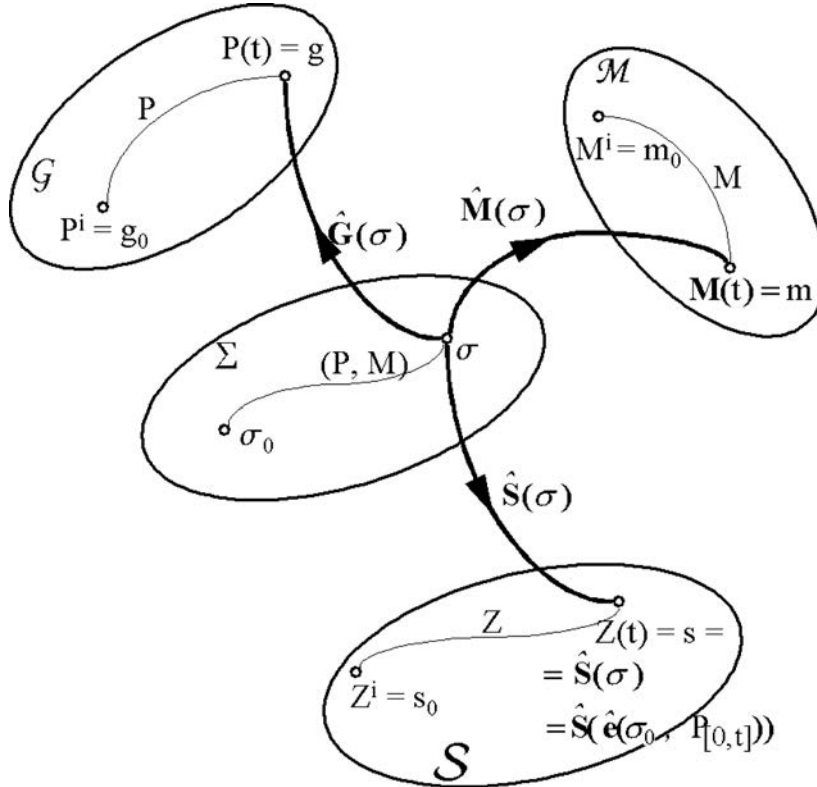


FIG. 3. Geometrical interpretation of mappings for a unique constitutive material structure.

The principle of determinism can be stated as follows: A unique value of the response  $s \in \mathcal{S}$  (i.e. unique values of the free energy  $\psi(t)$ , the entropy  $\eta(t)$ , the Kirchhoff stress tensor  $\tau$  and the heat flux vector  $\mathbf{q}(t)$ ) corresponds to every intrinsic state  $\sigma \in \Sigma$ .

The mapping  $\hat{\mathbf{S}}$  is called the response function (functional) or the constitutive function (functional).

**Definition 14.** The system  $(\mathcal{G}, \Pi, \Sigma, \hat{\mathbf{S}}, \hat{\mathbf{e}})$  is also a unique material structure in a particle  $X$  of a body  $\mathcal{B}$ .

<sup>9)</sup>It is noteworthy that both mappings  $\hat{\mathbf{e}}$  and  $\hat{\mathbf{S}}$  are similar to those introduced by NOLL [64] in a purely mechanical consideration but in the present theory, as in PERZYNA, KOSIŃSKI [96] and PERZYNA [77], the mappings  $\hat{\mathbf{e}}$  and  $\hat{\mathbf{S}}$  are generated by the constitutive mapping  $\mathfrak{R}$ .

The constitutive function  $\widehat{\mathbf{S}}$  and the evolution function  $\widehat{\mathbf{e}}$  will play a fundamental role in various descriptions of material constitutive structure. These descriptions will depend on different determination of the method of preparation space  $\mathcal{M}$ .

Recalling that a mapping  $\widehat{\mathbf{S}}$  determines the response of a material we can write

$$(3.29) \quad \widehat{\mathbf{S}} \equiv \{\widehat{\Psi}, \widehat{\mathbf{H}}, \widehat{\mathbf{T}}, \widehat{\mathbf{Q}}\},$$

where  $\widehat{\Psi}$  denotes the constitutive function of the free energy,  $\widehat{\mathbf{H}}$  the constitutive function of the entropy,  $\widehat{\mathbf{T}}$  the constitutive function of the Kirchhoff stress tensor and  $\widehat{\mathbf{Q}}$  the constitutive function of the heat flux vector.

### 3.6. Consequences of the dissipation principle

Taking account of Definition 2 we can state.

**Definition 15.** A local thermodynamical process  $\mathcal{P}_{\phi_t(B)} \subset \mathcal{P}_X$  compatible with a unique material structure  $(\mathcal{G}, \Pi, \Sigma, \widehat{\mathbf{S}}, \widehat{\mathbf{e}})$  will be called an admissible process.

A set of all admissible local thermodynamical processes we shall denote by  $\mathcal{P}_X^*$ .

**The principle of dissipation.** For every admissible local thermodynamical process the rate of entropy production in actual instant of time  $t \in [0, d_P]$  has nonnegative valued, i.e. the Clausius-Duhem inequality has to be satisfied, cf. COLEMAN, NOLL [19] and TRUESDELL [114]. The fundamental problem of the thermodynamics of materials is as follows: Within a set of admissible local thermodynamical processes  $\mathcal{P}_X^*$  and within a class of the constitutive functions  $\widehat{\mathbf{S}} = \{\widehat{\Psi}, \widehat{\mathbf{H}}, \widehat{\mathbf{T}}, \widehat{\mathbf{Q}}\}$  to determine those, which satisfy the dissipative principle. Thus, it can be said that the main problem of the thermodynamics of materials is the determination of an admissible local thermodynamical process.

It is noteworthy that the answer to the main problem of the thermodynamics of materials depends on the topology assumed for the method of preparation space.

It will be proved that the dissipation principle will imply two fundamental criteria in the theory of materials.

(i) The criterion of the selection of the response functions (functionals)  $\widehat{\mathbf{S}} = \{\widehat{\Psi}, \widehat{\mathbf{H}}, \widehat{\mathbf{T}}, \widehat{\mathbf{Q}}\}$ <sup>10</sup>.

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<sup>10</sup>It seems that ECKART [34] was the first who understood properly the consequences of the Clausius-Duhem inequality for constitutive assumptions. Further development of his idea was done by COLEMAN, NOLL [19], COLEMAN [16], COLEMAN, GURTIN [17], COLEMAN, MIZEL [18], COLEMAN, OWEN [20, 21] and TRUESDELL, NOLL [115].

(ii) The criterion of the accessibility of an intrinsic state  $\sigma \in \Sigma$  from the given initial intrinsic state  $\sigma_0 \in \Sigma^{11}$ .

3.7. Topological and smoothness assumptions

To investigate restrictions placed on a local thermodynamical process by the dissipation principle we assume:

1. The deformation-temperature configuration space  $\mathcal{G}$  and the method of preparation space  $\mathcal{M}$  are complete metrizable topological spaces (Banach spaces)<sup>12</sup>.
2. Processes  $P \in \Pi$  considered in the configuration space  $\mathcal{G}$  are continuous and continuously differentiable with respect to time  $t$ , i.e. for every  $t \in [0, d_P]$  exists the Lie derivative  $L_{\mathbf{v}}P(\tau)|_{\tau=t} = L_{\mathbf{v}}P(t)$ , which determines the rate of change of the process  $P$  at  $t$ .
3. Processes  $M$  determined in the method of preparation space  $\mathcal{M}$  are continuous and continuously differentiable with respect to time  $t$ , i.e. for every  $t \in [0, d_P]$  exists the Lie derivative  $L_{\mathbf{v}}M(\tau)|_{\tau=t} = L_{\mathbf{v}}M(t)$ , which determines the rate of change of the process  $M$  at  $t$ .
4. The rate  $L_{\mathbf{v}}M(t)$  is independent of the rate  $L_{\mathbf{v}}P(t)$  for every instant of time  $t \in [0, d_P]$ <sup>13</sup>.
5. The real value free energy response function  $\widehat{\Psi}$  defined on  $\Sigma \subset \mathcal{G} \times \mathcal{M}$  is continuously differentiable on  $\Sigma$ , i.e. the gradient  $\partial_{P(\tau)}\widehat{\Psi}|_{\tau=t}$  with fixed  $M(t)$  and the gradient  $\partial_{M(\tau)}\widehat{\Psi}|_{t=\tau}$  with fixed  $P(t)$  exist and are continuous functions on  $\Sigma$ . This property is called a chain rule property.

<sup>11</sup>The exploration of similar criterion to this has been taken, in another connection, by COLEMAN, OWEN [21].

<sup>12</sup>For the exact meaning of the mathematical terms introduced please consult KELLY [48] and ENGELKING [35].

<sup>13</sup>Since the rate  $L_{\mathbf{v}}M(t)$  is independent of the rate  $L_{\mathbf{v}}P(t)$ , then we may postulate

$$(*) \quad L_{\mathbf{v}}M(t) = \widehat{\mathcal{M}}(P(t), M(t)), \quad t \in [0, d_P].$$

Under this assumption the rate of change of the process  $M(t)$  in the method of preparation space  $\mathcal{M}$  is completely determined by the actual intrinsic state  $\sigma \in \Sigma$ .

Two interesting cases can be considered:

- (i)  $M(0) = m_o \in \mathcal{M}$ ,
- (ii)  $M(-\infty) = m_{-\infty} \in \mathcal{M}$ .

The differential equation (\*) is called the evolution equation in the method of preparation space  $\mathcal{M}$ , and together with appropriate initial value (i) or (ii) for the given deformation-temperature configuration process  $P : [0, d_P] \rightarrow \mathcal{G}$  completely determines the evolution of the intrinsic state, i.e. the evolution function  $\widehat{\mathbf{e}} : (\Sigma \times \Pi)^* \rightarrow \Sigma$ .

The differential equation (\*) with the initial value (i) leads to the unique material structure with internal state variables, and the initial value problem (\*) and (ii) is isomorphic with the unique material structure with memory, cf. KOSIŃSKI, WOJNO [50] and LEITMAN, MIZEL [56].

Since  $\mathcal{G}$  and  $\mathcal{M}$  have been normed spaces (Banach spaces), then it has been more convenient to consider a subset  $\mathcal{D}$  of the intrinsic state space  $\Sigma$ , being the complete normed space (Banach space). We shall assume that the constitutive functions (functionals)  $\widehat{\mathbf{S}} \equiv \{\widehat{\Psi}, \widehat{\mathbf{H}}, \widehat{\mathbf{T}}, \widehat{\mathbf{Q}}\}$  are defined on a set  $\mathcal{D}$ .

To speak precisely, a property of chain rule for the constitutive function (functional) of the free energy  $\widehat{\Psi}$  is assumed in the topology of  $\mathcal{D}$ .

### 3.8. Constitutive restriction

Thanks to previous assumptions, from the satisfaction of the dissipative principle in the form of the Clausius-Duhem inequality (3.6), we receive the results as follows<sup>14)</sup>

$$(3.30) \quad \begin{aligned} \partial_{\text{grad}\vartheta(t)} \widehat{\Psi}(\cdot) &= 0, & \boldsymbol{\tau}(t) &= \rho_{\text{Ref}} \partial_{\mathbf{e}(t)} \widehat{\Psi}(\cdot), & \eta(t) &= -\partial_{\vartheta(t)} \widehat{\Psi}(\cdot), \\ -\partial_{M(t)} \widehat{\Psi}(\cdot) \square \mathbf{L}_{\mathbf{v}} M(t) - \frac{1}{\rho\vartheta(t)} \widehat{\mathbf{Q}}(\cdot) \cdot \text{grad}\vartheta(t) &\geq 0, \end{aligned}$$

valid at every instant of time  $t \in [0, d_P]$ . The expression  $\partial_{M(t)} \widehat{\Psi}(\cdot) \square \mathbf{L}_{\mathbf{v}} M(t)$  denotes the product of two geometrical objects with full contraction. Let us introduce the following denotations

$$(3.31) \quad \begin{aligned} \widehat{d}(\sigma) &= -\partial_{M(t)} \widehat{\Psi}(\cdot) \square \mathbf{L}_{\mathbf{v}} M(t) - \frac{1}{\rho\vartheta(t)} \widehat{\mathbf{Q}}(\cdot) \cdot \text{grad}\vartheta(t), \\ \widehat{i}(\sigma) &= -\frac{1}{\vartheta(t)} \partial_{M(t)} \widehat{\Psi}(\cdot) \square \mathbf{L}_{\mathbf{v}} M(t). \end{aligned}$$

The mapping  $\widehat{d} : \Sigma \rightarrow \mathbf{R}^+$  (where  $\mathbf{R}^+$  denotes the set of non-negative real numbers) is called the general dissipation function, and  $\widehat{d}(\sigma)$  denotes the value of the general dissipation function at the intrinsic state  $\sigma \in \Sigma$ .

The mapping  $\widehat{i} : \Sigma \rightarrow \mathbf{R}^+$  is called the internal dissipation function, and  $\widehat{i}(\sigma)$  is its value at the intrinsic state  $\sigma \in \Sigma$ .

The inequality (3.30)<sub>4</sub> is called the general dissipation inequality and using the denotations (3.31), it can be written in the form

$$(3.32) \quad \widehat{d}(\sigma) = \vartheta(t) \widehat{i}(\sigma) - \frac{1}{\rho\vartheta(t)} \widehat{\mathbf{Q}}(\sigma) \cdot \text{grad}\vartheta(t) \geq 0.$$

The results (3.30) express the criterion of the selection of the response functions (functionals)  $\widehat{\mathbf{S}} \equiv \{\widehat{\Psi}, \widehat{\mathbf{H}}, \widehat{\mathbf{T}}, \widehat{\mathbf{Q}}\}$ , which can be stated as follows:

<sup>14)</sup>To prove this statement we can use a similar procedure to that of COLEMAN, GURTIN [17] and VALANIS [116].



Choosing the free energy constitutive function  $\widehat{\Psi}(\cdot)$  which is independent of the actual temperature gradient  $\text{grad}\vartheta(t)$  and the heat flux response function  $\widehat{\mathbf{Q}}(\cdot)$  such that the general dissipation inequality (3.32) is satisfied at every instant of time  $t \in [0, d_P]$ , or for every intrinsic state  $\sigma$  determined by the relation  $\sigma = \widehat{\mathbf{e}}(\sigma_0, P_{[0,t]})$ , where  $\sigma_0$  denotes the initial intrinsic state and  $P_{[0,t]}$  the segment of the given deformation-temperature process  $P$ , the response Kirchhoff stress function  $\widehat{\mathbf{T}}$  and the response entropy function  $\widehat{\mathbf{H}}$  are uniquely determined by the relations (3.30)<sub>2</sub> and (3.30)<sub>3</sub>. It is noteworthy that for the adiabatic thermodynamical process, when  $\mathbf{q}(t) \equiv 0$  or  $\text{grad}\vartheta(t) \equiv 0$  for  $t \in [0, d_P]$  the general dissipation inequality (3.32) takes the particular form

$$(3.33) \quad \widehat{i}(\sigma) = -\frac{1}{\vartheta(t)} \partial_{M(t)} \widehat{\Psi}(\cdot) \square L_{\mathbf{v}} M(t) \geq 0, \quad t \in [0, d_P]$$

which is called the internal dissipation inequality.

### 3.9. Accessibility criterion

Let us assume that the initial intrinsic state  $\sigma_0 \in \Sigma$  is known, and let us choose an arbitrary intrinsic state  $\sigma^* \in \Sigma$ . The question arises whether the intrinsic state  $\sigma^*$  is accessible from the initial intrinsic state  $\sigma_0$ , or in other words, what is the condition of accessibility of  $\sigma^*$  from  $\sigma_0$ .

If the intrinsic state  $\sigma^*$  is accessible from the initial intrinsic state  $\sigma_0$ , then the deformation-temperature process  $P$  has to exist which generates the process in the method of preparation space  $M : [0, d_P] \rightarrow \mathcal{M}$  such that

$$(3.34) \quad \begin{aligned} \sigma_0 &= (P(0), M(0)) = (g_0, m_0), \\ \sigma^* &= (P(d_P), M(d_P)) = (g^*, m^*) \end{aligned}$$

and for every instant of time  $t \in [0, d_P]$  the dissipation principle is satisfied. The response of a material corresponding to the intrinsic state  $\sigma^*$  is determined by the constitutive relation

$$(3.35) \quad Z(d_P) = \widehat{\mathbf{S}}(\widehat{\mathbf{e}}(\sigma_0, P)) = \widehat{\mathbf{S}}(\sigma^*).$$

The dissipation principle requires that for a given process  $P$  such a process  $M : [0, d_P] \rightarrow \mathcal{M}$  be chosen that the general dissipation inequality

$$(3.36) \quad \widehat{d}(\sigma) \geq 0, \quad \sigma = (P(t), M(t)) = (g, m)$$

for every instant of time  $t \in [0, d_P]$  has to be satisfied.

**Accessibility criterion of the intrinsic states.** An arbitrary intrinsic state  $\sigma^* \in \Sigma$  is accessible from the initial intrinsic state  $\sigma_0 \in \Sigma$  if there exists a pair of processes  $(P, M) : [0, d_P] \rightarrow \mathcal{G} \times \mathcal{M}$  such that the following conditions are satisfied:

$$(3.37) \quad (i) \quad (P(0), M(0)) = (g_0, m_0) = \sigma_0, \quad (P(d_P), M(d_P)) = (g^*, m^*) = \sigma^*,$$

$$(3.38) \quad (ii) \quad \widehat{d}(\sigma) = \widehat{d}(\widehat{\mathbf{e}}(\sigma_0, P_{[0,t]})) \geq 0 \quad \text{for every instant of time } t \in [0, d_P].$$

It is noteworthy that the accessibility criterion places some restrictions on the evolution function  $\widehat{\mathbf{e}} : (\Sigma \times \Pi)^* \rightarrow \Sigma$ .

### 3.10. Principle of the increase of entropy

Let us consider the intrinsic state space  $\Sigma$ . In this space we choose the initial intrinsic state  $\sigma_0$  and an arbitrary intrinsic state  $\sigma$ . Let us assume that there exists a pair of processes  $(P, M) : [0, d_P] \rightarrow \mathcal{G} \times \mathcal{M}$  such that

$$(3.39) \quad \begin{aligned} (P(0), M(0)) &= (g_0, m_0) = \sigma_0, \\ (P(t), M(t)) &= (g, m) = \sigma. \end{aligned}$$

The pair of the processes  $(P, M)$  is represented in the intrinsic state space  $\Sigma$  by the curve  $\mathcal{L}$ .

We define the curvilinear integral along the curve  $\mathcal{L}$ , which due to natural time parametrization can be written in the form

$$(3.40) \quad J(\sigma_0, \sigma) = \int_0^t \widehat{d}(P(\tau), M(\tau)) d\tau = \int_0^t \widehat{d}(\widehat{\mathbf{e}}(\sigma_0, P_{[0,\tau]})) d\tau, \quad t \in [0, d_P].$$

In a similar way we can define the integral

$$(3.41) \quad I(\sigma_0, \sigma) = \int_0^t \widehat{i}(P(\tau), M(\tau)) d\tau = \int_0^t \widehat{i}(\widehat{\mathbf{e}}(\sigma_0, P_{[0,\tau]})) d\tau, \quad t \in [0, d_P].$$

The integrals  $J(\sigma_0, \sigma)$  and  $I(\sigma_0, \sigma)$  are called the general dissipation integral and the internal dissipation integral, respectively.

Let us consider in the intrinsic state space  $\Sigma$  two intrinsic states  $\sigma_a$  and  $\sigma_b$ , which lie on the curve  $\mathcal{L}$ . The intrinsic state  $\sigma_a$  corresponds to the instant of time  $t_a \in [0, d_P]$  and the intrinsic state  $\sigma_b$  to the instant of time  $t_b \in [0, d_P]$ , and of course  $t_b > t_a$ .

The dissipation principle requires that

$$(3.42) \quad J(\sigma_0, \sigma_b) - J(\sigma_0, \sigma_a) \geq 0.$$

**Principle of the increase of entropy:** For all  $\sigma_a, \sigma_b \in \Sigma$ ,  $\sigma_b$  is accessible from  $\sigma_a$  if, and only if, the general dissipation integral of  $\sigma_b$  is not less than that of  $\sigma_a$ .

It is important to note that the internal dissipation integral (3.41) is a measure of the irreversibility of a local thermodynamical process for the case when  $\mathbf{q}(t) \equiv 0$  or  $\nabla\vartheta(t) \equiv 0$  for  $t \in [0, d_P]$  (i.e. for an adiabatic process), and may be interpreted as the empirical entropy<sup>15)</sup> or as the irreversibility function<sup>16)</sup>.

If we assume this interpretation and the condition  $\mathbf{q}(t) \equiv 0$  for  $t \in [0, d_P]$  we can state the principle of increase of entropy in the form as follows (cf. RASTALL [105]): For all  $\sigma_a, \sigma_b \in \Sigma$ ,  $\sigma_b$  is adiabatically accessible from  $\sigma_a$  if, and only if, the empirical entropy of  $\sigma_b$  is not less than that of  $\sigma_a$ .

The principle of the increase of entropy was first formulated by PLANCK [101, 102].

It is worth pointing out on some features of the thermodynamics of materials presented. We started from the dissipation principle in the form of the Clausius-Duhem inequality and we deduced two fundamental criteria for the thermodynamics of materials, namely the criterion of the selection of the response functions (functionals) occurring in the mathematical statement of the general principle of determinism and the accessibility criterion in the intrinsic state space  $\Sigma$ .

The accessibility criterion is connected with the Caratheodory formulation of the second law of thermodynamics, cf. CARATHEODORY [14]<sup>17)</sup>.

As a consequence of the dissipation principle we also deduced the principle of the increase of entropy. Appropriate interpretation of the general dissipation integral (or the internal dissipation integral) led to the very old statement of the second law of thermodynamics first presented by PLANCK [101, 102]<sup>18)</sup>.

It is noteworthy to stress that all considerations concerned a general unique material structure before a particular realization of the method of preparation had been assumed.

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<sup>15)</sup>The clear meaning of the empirical entropy can be found in the papers by BUCHDAHL [10, 11], cf. also BUCHDAHL, GREVE [12], COOPER [22], RASTALL [105] and BOYLING [7, 8].

<sup>16)</sup>The concept of the irreversibility function was introduced by GILES [39].

<sup>17)</sup>Caratheodory's formulation of classical thermodynamics has been developed further by BORN [6], BUCHDAHL [10, 11], FALK, JUNG [36], BERNSTEIN [4], BUCHDAHL, GREVE [12], LANDSBERG [52, 53, 54], COOPER [22], RASTALL [105] and BOYLING [7, 8].

<sup>18)</sup>Extension of Planck's idea has been done by BUCHDAHL [10], RASTALL [105] and BOYLING [7, 8].

## 4. INTERNAL STATE VARIABLE MATERIAL STRUCTURE

## 4.1. Fundamental assumptions

**Proposition 1.** The method of preparation space for the element body with a unique material structure  $(\mathcal{G}, \Pi, \Sigma, \mathfrak{R})$  is a finite dimensional vector space  $\mathcal{W}$ , i.e.

$$(4.1) \quad \mathcal{M} = \mathcal{W},$$

and the intrinsic state space  $\Sigma$  is the set

$$(4.2) \quad \Sigma \equiv \{(g, m) \mid g \in \mathcal{G}, \quad m \in \mathcal{W}_g, \quad \overline{\overline{\mathcal{W}}}_g = \overline{\overline{\mathcal{Z}}}_P\},$$

where  $P \in \Pi_g$ .

Elements of the method of preparation space  $m \in \mathcal{W}$  are vectors. Components of the vector  $m \in \mathcal{W}$  are called the internal state variables.

**Proposition 2.** Let us assume that such a mapping exists

$$(4.3) \quad \widehat{\mathcal{M}} : \Sigma \rightarrow \mathcal{W},$$

that for every  $P \in \Pi$  and  $m_0 \in \mathcal{W}_{P_i}$  the initial value problem

$$(4.4) \quad L_{\mathbf{v}} M(t) = \widehat{\mathcal{M}}(P(t), M(t)), \quad M(0) = m_0$$

has the unique solution  $M : [0, d_P] \rightarrow \mathcal{W}$ .

The constitutive mapping  $\mathfrak{R} : (\Sigma \times \Pi)^* \rightarrow \mathcal{Z}$  has to satisfied the condition

$$(4.5) \quad \mathfrak{R}(\widehat{\mathcal{G}}(\sigma), \cdot, P) : \mathcal{W}_{P_i} \rightarrow \mathcal{Z}_P \quad \text{must be bijection}$$

for arbitrary  $(\sigma, P) \in (\Sigma \times \Pi)^*$ .

The evolution function  $\widehat{\mathbf{e}} : (\Sigma \times \Pi^*) \rightarrow \Sigma$  is generated by the constitutive mapping  $\mathfrak{R}$  and has the form

$$(4.6) \quad \widehat{\mathbf{e}}(\sigma, P) = (P^f, \mathcal{F}_{d_P}(P, \widehat{\mathcal{M}}(\sigma))),$$

where  $\mathcal{F}$  denotes the solution functional of the initial value problem (4.4), i.e.

$$(4.7) \quad M(t) = \mathcal{F}_t(P, \widehat{\mathcal{M}}(\sigma)).$$

Equation (4.4)<sub>1</sub> is called the evolution equation for the internal state variable vector  $m$ , and  $\widehat{\mathcal{M}}$  is called the method of preparation evolution function.

The principle of determinism for the material structure with internal state variables can be written as follows

$$(4.8) \quad Z(t) = s = \widehat{\mathbf{S}}(\sigma), \quad \sigma = (P(t), M(t)) = (g, m),$$

or by using the evolution function in the form

$$(4.9) \quad Z(t) = \widehat{\mathbf{S}}(\widehat{\mathbf{e}}(\sigma_0, P_{[0,t]})), \quad \sigma_0 = (g_0, m_0).$$

This principle of determinism can be expressed as follows: Transient value of the deformation-temperature configuration and transient value of the internal state variable vector determine the unique transient value of the reaction at a particle X in a body  $\mathcal{B}$ .

4.2. Investigation of the thermodynamical restrictions

The function  $\widehat{\mathbf{S}}$  represents the constitutive functions  $\widehat{\Psi}$ ,  $\widehat{\mathbf{H}}$ ,  $\widehat{\mathbf{T}}$ ,  $\widehat{\mathbf{Q}}$ . The domain of the constitutive functions is a subset of the intrinsic state  $\Sigma = \mathcal{G} \times \mathcal{W}$ . Since the method of preparation space  $\mathcal{W}$  is a finite dimensional vector space and the deformation-temperature configuration space is also a finite dimensional space, hence the intrinsic state space  $\Sigma$  is the complete normed space (Banach space). Assuming the conditions 2–5 of Section 3 we have the results (3.30)<sub>1–3</sub> valid for the material structure with the internal state variables, and the general dissipation inequality (3.30)<sub>4</sub> takes the form

$$(4.10) \quad \widehat{d}(\sigma) = -\partial_{M(t)}\widehat{\Psi}(\cdot) \cdot L_v M(t) - \frac{1}{\rho\vartheta(t)}\widehat{\mathbf{Q}}(\cdot) \cdot \text{grad}\vartheta(t) \geq 0.$$

The internal dissipation function  $\widehat{i} : \Sigma \rightarrow \mathbb{R}^+$  for this material structure is determined by

$$(4.11) \quad \widehat{i}(\sigma) = -\frac{1}{\vartheta(t)}\partial_{M(t)}\widehat{\Psi}(\cdot) \cdot L_v M(t).$$

Taking advantage of the evolution equation (4.4)<sub>1</sub> we have

$$(4.12) \quad \widehat{i}(\sigma) = -\frac{1}{\vartheta(t)}\partial_{M(t)}\widehat{\Psi}(\cdot) \cdot \widehat{\mathcal{M}}((P(t), M(t))).$$

Now we can return to the discussion of the notion of the method of preparation as such information which is required for the description of the internal dissipation of an inelastic material. The expression (4.12) which defines the value of the internal dissipation function at the intrinsic state  $\sigma$  shows that full information given in the method of preparation, i.e.  $M(t) = m$  and the evolution function  $\widehat{\mathcal{M}}$ , essentially determines the rate of internal dissipation for this intrinsic state  $\sigma$ . This conclusion is of fundamental importance for the physical interpretation of the internal state variables. Indeed, the internal dissipation in this conception is a key for this interpretation.

**Definition 15.** The body element with a unique material structure  $(\mathcal{G}, \Pi, \Sigma, \widehat{\mathbf{S}}, \widehat{\mathbf{e}})$  satisfying the **Proposition 1 and 2** is called the material structure with internal state variables.

The using of the conception of the internal state variables for the mechanics of continuous media was proposed by COLEMAN, GURTIN [17]. In the theory of elasto-viscoplasticity this idea has been applied for the first time by PERZYNA, WOJNO [98], cf. also PERZYNA [72, 73, 75, 76, 77, 81] and PERZYNA, WOJNO [99].

## 5. THERMODYNAMICAL THEORY OF ELASTO-VISCOPLASTICITY

### 5.1. *Physical foundations and experimental motivations*

#### 5.1.1. *Physical origin of elastic-viscoplastic response of a material of solids*

The high-rate deformation of face-centered cubic (f.c.c.) metals, such as copper, aluminum, lead and nickel has been recently extensively studied (cf. review paper by FOLLANSBEE [38]). It has been shown that the apparent strain rate sensitivity of f.c.c. metals has two origins: that associated with the finite velocity of dislocations, and that connected with the evolution of the dislocation substructure. The first of these two components – the instantaneous rate sensitivity – is related to the wait-times associated with thermally activated dislocation motion. The second component has more to do with the relative importance of dislocation generation and annihilation at different strain rates, and shall be referred to as the strain rate history effect.

The rate and temperature dependence of the flow stress of metal crystals can be explained by different physical mechanisms of dislocation motion. The microscopic processes combine in various ways to give several groups of deformation mechanisms, each of which can be limited to the particular range of temperature and strain rate changes, cf. PERZYNA [91].

It will be profitable for further considerations to discuss the interaction of the thermally activated and phonon dumping mechanisms.

5.1.2. *Interaction of the thermally activated and phonon damping mechanisms* If a dislocation is moving through the rows of barriers, then its velocity can be determined by the expression (cf. Fig. 4)

$$(5.1) \quad v = AL^{-1}/(t_S + t_B),$$

where  $AL^{-1}$  is the average distance of dislocation movement after each thermal activation,  $t_S$  is the time a dislocation spent at the obstacle, and  $t_B$  is the time of travelling between the barriers.

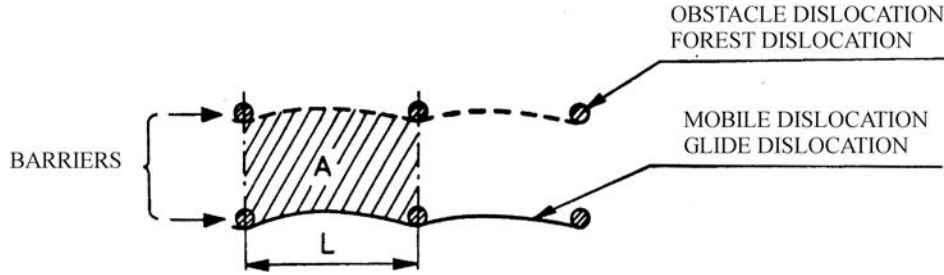


FIG. 4. Intersection of forest dislocations.

The shearing rate in single slip is given by the relationship (cf. SEEGER [108, 109, 110], KUMAR, KUMBLE [51], TEODOSIU, SIDOROFF [113] and PERZYNA [79, 85, 90, 91])

$$(5.2) \quad \dot{\epsilon}^p = \frac{1}{T_{mT}} \langle \exp \{ U [ (\tau - \tau_\mu) L b ] / k \vartheta \} + B A L^{-1} \nu / (\tau - \tau_B) b \rangle^{-1},$$

where  $U$  is the activation energy (Gibbs free energy),  $b$  denotes the Burgers vector,  $k$  is the Boltzman constant,  $\vartheta$  actual absolute temperature,  $B$  denotes the dislocation drag coefficient,  $\nu$  is the frequency of vibration of the dislocation,  $\tau_\mu$  denotes the athermal stress and  $\tau_B$  is attributed to the stress needed to overcome the forest dislocation barriers to the dislocation motion and is called the back stress.

The two relaxation times

$$(5.3) \quad \frac{1}{T_{mT}} \frac{b \tau_B}{B A L^{-1} \nu} = \frac{\alpha b^2 \tau_B}{B} = \frac{1}{T_{mD}},$$

and two effective resolved shear stresses

$$(5.4) \quad \tau_T^* = \tau - \tau_\mu \quad \text{and} \quad \tau_D^* = \tau - \tau_B$$

are separately defined for the thermally activated and phonon damping mechanisms, respectively.

If the time  $t_B$  taken by the dislocation to travel between the barriers in a viscous phonon medium is negligible when compared with the time  $t_S$  spent at the obstacle, then

$$(5.5) \quad v = \frac{A L^{-1}}{t_S}$$

and we can focus our attention on the analysis of the thermally activated process.

When the ratio  $t_B/t_S$  increases then the dislocation velocity (5.1) can be approximated by the expression

$$(5.6) \quad v = \frac{AL^{-1}}{t_B}$$

for the phonon damping mechanism.

It is noteworthy to stress that the relaxation time varies when the mechanism of the dislocation motion changes from the thermally activated to the phonon damping.

Experimental justifications of the thermally activated and phonon damping mechanisms as well as the discussion of their range rate and temperature changes for particular materials have been given in many papers. Particular importance for our purposes have results obtained by CAMPBELL, FERGUSON [13]. In their paper an account is given of experiments in which the shear flow stress of mild steel was measured at temperature from 195 to 713 K and strain rate from  $10^{-3}$  to  $4 \cdot 10^4 \text{ s}^{-1}$ . The flow stress at lower yield is plotted in Fig. 5 as shear stress against the logarithm of shear strain rate, for the various temperatures used throughout the investigation.

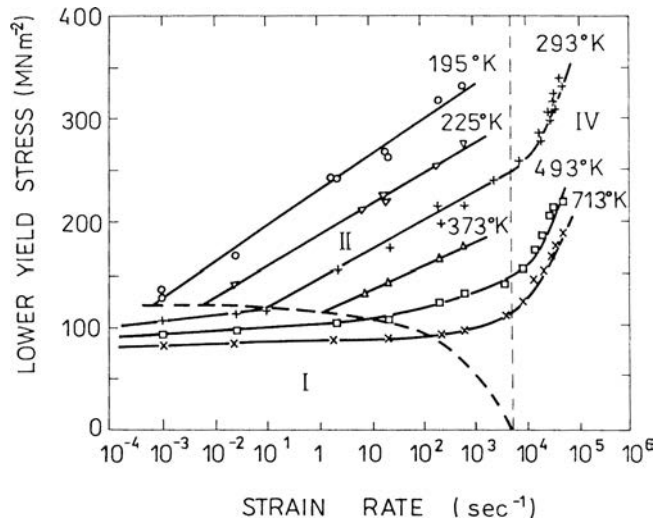


FIG. 5. Variation of lower yield stress with strain rate, at constant temperature.  
After CAMPBELL, FERGUSON [13].

For the purpose of the discussion which follows, it is convenient to divide the curves into three regions, each corresponding to a certain range of strain rate which is a function of the temperature. Following ROSENFELD, HAHN [106] these will be referred to as region I, II and IV. These regions are indicated in Fig. 5, cf. also Fig. 6.



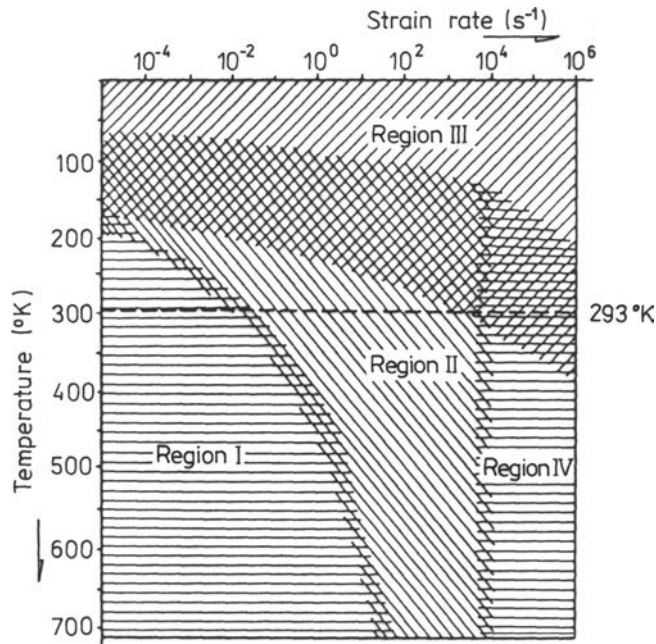


FIG. 6. Regions of the temperature strain rate spectrum of low carbon steel that reflect different mechanisms of yielding. After ROSENFELD, HAHN [106] and CAMPBELL, FERGUSON [13].

In region I the flow stress shows a small temperature and strain rate sensitivity, the latter decreasing with increasing temperature. Prestraining increases the flow stress but has little effect on the rate sensitivity of the flow stress,  $(\partial\tau/\partial \ln \dot{\epsilon}^p)_\theta$ , at room temperature, cf. Fig. 7. The dominant factor in region I seems to be the long-range internal stress fields due to dislocations, precipitate particles, grain boundaries etc.

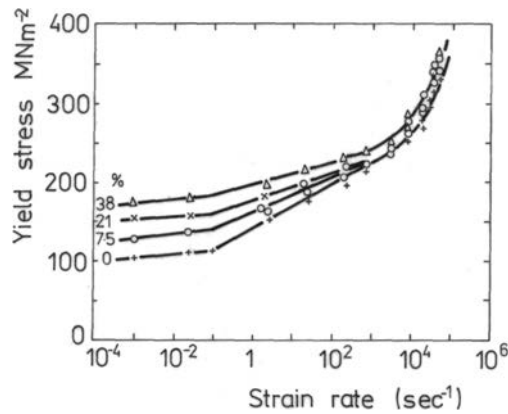


FIG. 7. Effect of pre-straining on variations of yield stress with strain rate. After CAMPBELL, FERGUSON [13].

In region II the flow stress shows greater rate and temperature sensitivities. From a survey of their own and previous work, ROSENFELD, HAHN [106] concluded that in this region the rate sensitivity  $(\partial\tau/\partial \ln \dot{\epsilon}^p)_\vartheta$  is independent of temperature and strain rate. However, the data of CAMPBELL, FERGUSON [13] show a consistent increase in  $(\partial\tau/\partial \ln \dot{\epsilon}^p)_\vartheta$  as temperature is reduced.

It has been suggested by CAMPBELL, FERGUSON [13] that the flow behaviour throughout region II can be explained by the thermal activation of dislocation motion.

Since the relaxation time  $T_m T$  is related to the dislocation structure it may be governed by the deformation history, rather than a function of the state variables  $\epsilon^p$ ,  $\tau$  and  $\vartheta$ .

The experimental data obtained by CAMPBELL, FERGUSON [13] for mild steel in region II are properly interpreted by the linear approximation of the thermally activated theory.

Region IV is characterized by a rapid increase in semi-logarithmic rate sensitivity  $(\partial\tau/\partial \ln \dot{\epsilon}^p)_\vartheta$  with increasing strain rate, this parameter being approximately independent of temperature in the range 293 to 713 K.

In Fig. 8 the experimental data of CAMPBELL, FERGUSON [13] for region IV are replotted using a linear strain-rate scale, and it is seen that, within the accuracy of measurement, they can be represented by straight lines at all three temperatures and all three values of pre-strain. While the slopes of these lines show only a small dependence on temperature, their intercepts on the stress axis vary greatly with temperature.

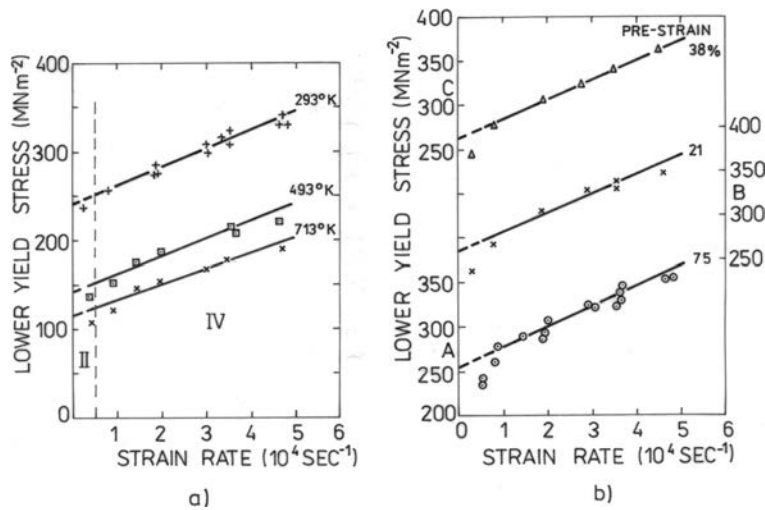


FIG. 8. Variation of lower yield stress with strain rate (region IV). (a) Zero pre-strain; temperature 293, 493, 713 K. (b) Pre-strain 7.5, 21, 38%; temperature 293 K. After CAMPBELL, FERGUSON [13].

*5.1.3. Microshear banding effects* Basing on the analysis of dynamical experimental observations for single crystals and polycrystalline metals (cf. PERZYNA [92]) we can conclude that microshear banding influences very much a substructure of a material under consideration. As a result of this it contributes mainly to viscoplastic strain rate effects.

For the elastic-viscoplastic model of polycrystalline solids the relaxation time  $T_m$  governs the viscoplastic flow in the entire range of strain rate changes and for classical models it is generally assumed as constant value. However, in real case it has to be a function of the rate of equivalent inelastic deformation  $\dot{\epsilon}^P$  and the active microshear bands fraction  $f_{ms}$  (cf. NOWAK *et al.* [67], PERZYNA [92]).

For the description of plastic deformation of polycrystalline metals accounting for the effects of microshear bands please consult paper by PEŁCHERSKI [100].

*5.1.4. Induced anisotropy effects* For our considerations of anisotropic effects, the metallurgical aspects of fracture and spalling have great importance. Effects of parameters such as grain size and substructure, crack/void initiation sites, micromechanical aspects of growth, and coalescence can influence fracture and spalling mechanisms.

There are essentially two modes of dynamic fracture: ductile and brittle. Ductile fracture is characterized by voids which, in spalling, tend to be spherical up to a certain size. Brittle fracture shows cracks with sharp tips at which fracture proceeds with relatively little plastic deformation. FCC metals exhibit a higher ductility at high strain rates and tend to spall in a ductile manner. BCC and HCP metals tend to spall by a brittle mode.

It is generally accepted that the intrinsic microdamage process consists of nucleation, growth and coalescence of microcracks (microvoids). Microfracture nucleation is classified into homogeneous and heterogeneous. Homogeneous nucleation takes place when thermal energy fluctuations is assisted (cf. MEYERS, AIMONE [60]). Heterogeneous nucleation is realized as the result of fracture of inclusions or second-phase particles, separation of interfaces, fracture of the matrix and fracture at grain boundaries, cf. Figs. 9, 10 and 11.

To show the complexity of the anisotropy phenomena in microdamage process we shall discuss several available experimental results.

The most popular dynamical experiment<sup>19)</sup> in the investigation of the fracture phenomenon in metals is a plate-impact configuration system. This experimental system consists of two plates, a projectile plane plate impacts against

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<sup>19)</sup>For a thorough discussion of the experimental and theoretical works in the field of dynamic fracture and spalling of metals please consult the review papers by MEYERS, AIMONE [60] and CURRAN *et al.* [25], cf. also MEYERS [59].

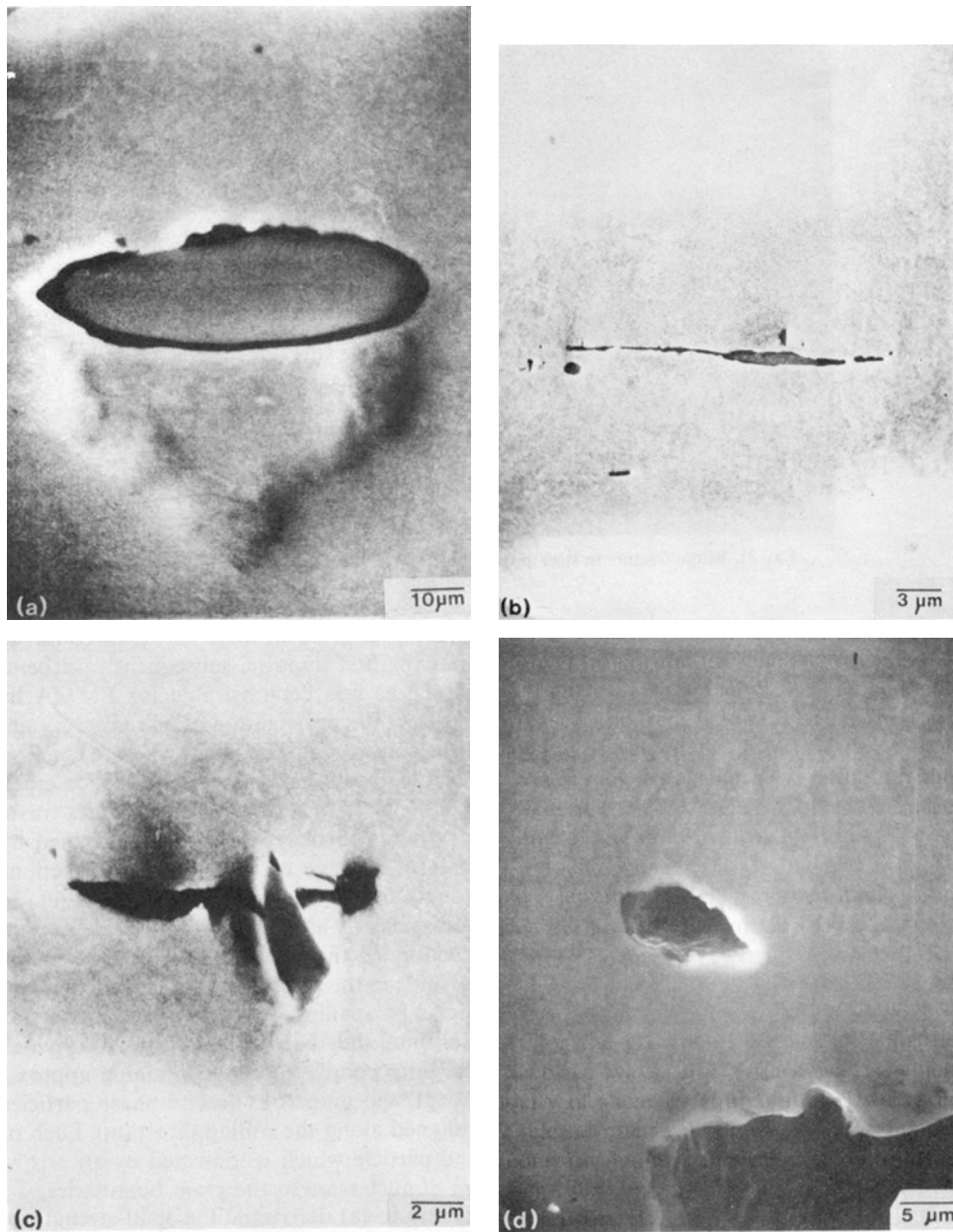


FIG. 9. Four different sources of spall initiation in steel. (a) Debonding at MnS – matrix interface; (b) crack starting at MnS and propagating into matrix; (c) crack starting at silicate interface and propagating into matrix; (d) void apparently homogeneously generated (After SHOCKEY *et al.* [111]).

a target plane. This is a good example of a dynamic deformation process. If impact velocity is sufficiently high the propagation of a plastic wave through

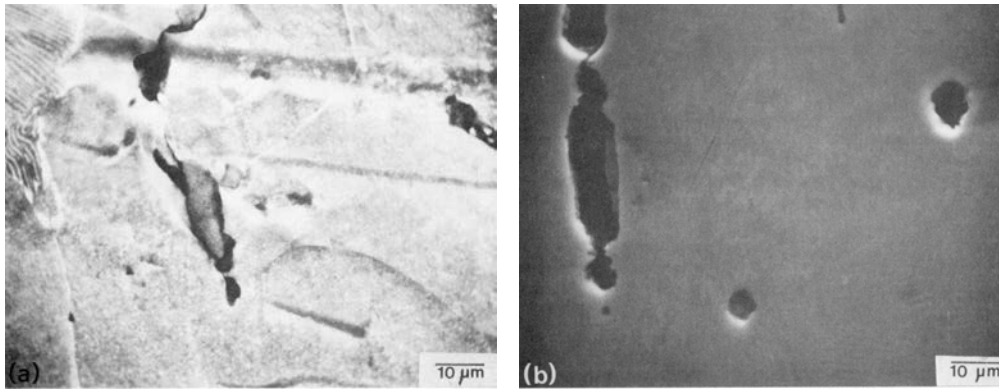


FIG. 10. Two incidences of fracture initiation at MnS – matrix interface in steel. In (b) fracture propagates in a ductile manner, by void nucleation and growth (After SHOCKEY *et al.* [111]).

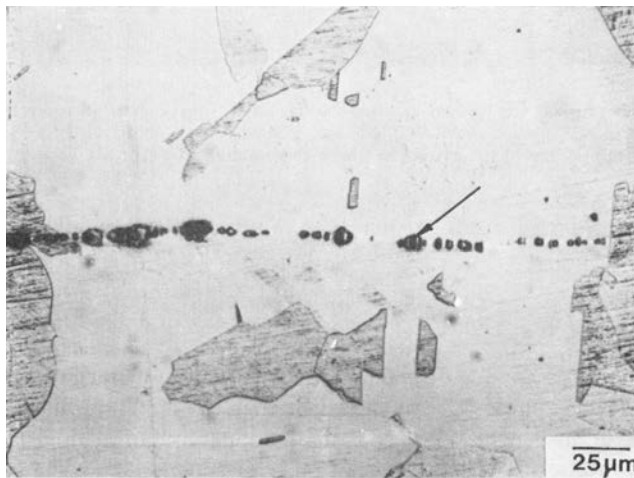


FIG. 11. Formation of a string of voids by nucleation at second-phase particles in nickel. Some second-phase particles that are fractured can be seen (After SHOCKEY *et al.* [111]).

the target is generated. The reflection and interaction of waves result a net tensile pulse in the target plate. If this stress pulse has sufficient amplitude and sufficient time duration, it will cause separation of the material and spalling process.

The reason for choosing this particular kind of dynamical experiment is that postshot photomicrographic observations of the residual porosity are available, and the stress amplitude and pulse duration can be performed sufficiently great to produce substantial porosity and the spall of the target plate.

The experimental data presented by SEAMAN *et al.* [107] illustrate damage phenomena and provide a common basis for considering damage criteria. They

have used a plate-impact configuration system. Following the compression waves resulting from the impact, rarefaction waves have intersected near the middle of the target plate to cause damage in the form of nearly spherical voids. The heaviest damage is localized in a narrow zone, which is called the spall plane. Both the number and the size of voids decrease with distance from this zone. This type of damage is termed ductile fracture because of high ductility (ability to flow) required of the plate material, Fig. 12.

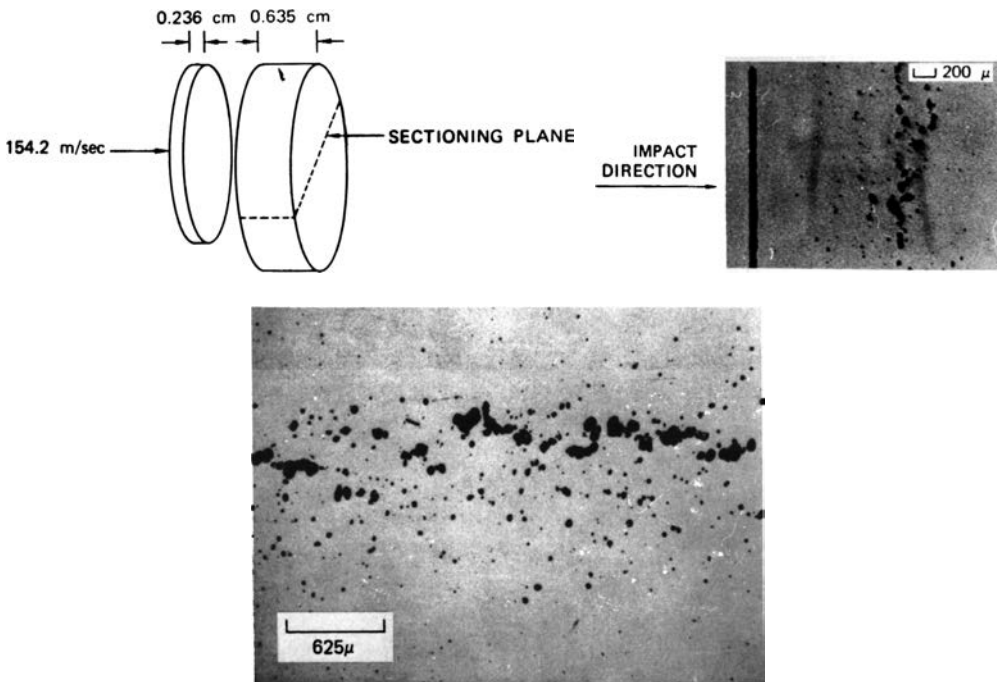


FIG. 12. A cross section of an aluminium target plate that has undergone a planar impact by another aluminium plate (After SEAMAN *et al.* [107]).

The final damage of the target plate (aluminium 1145) for a constant shot geometry but for different impact velocities has been performed by BARBEE *et al.* [3]. The results suggest dependence of spalling process on the pulse amplitude, Fig. 13.

A sample of full separation is shown in Fig. 14, an aluminium target impacted by a plate has been damaged to the extent that full separation occurred near the center of the target, cf. SEAMAN *et al.* [107]. The authors suggested that this full separation appears as a macrocrack propagating through heavily damaged material. The macrocrack occurs as a result of coalescence of microvoids which is also visible in Fig. 14.

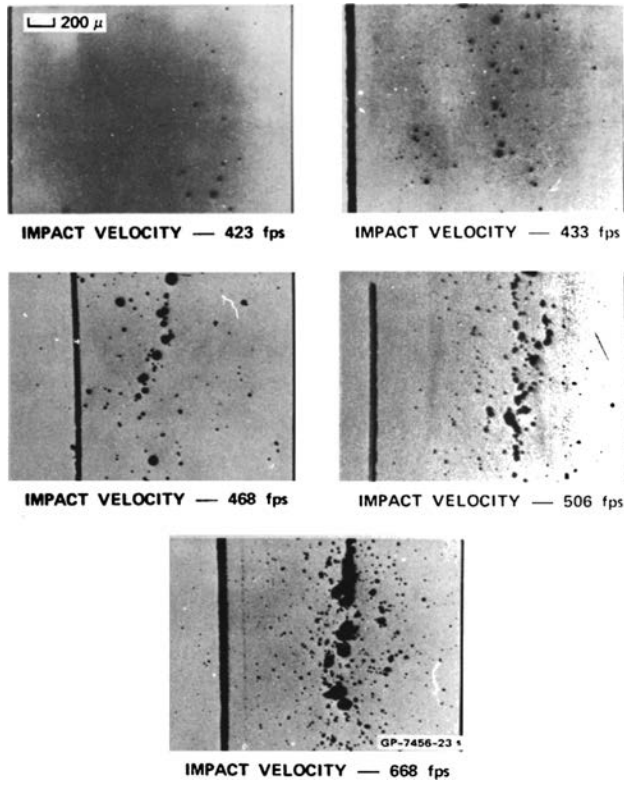


FIG. 13. The final damage of the aluminum 1145 target plate for a constant shot geometry but for different impact velocities (After BARBEE *et al.* [3]).

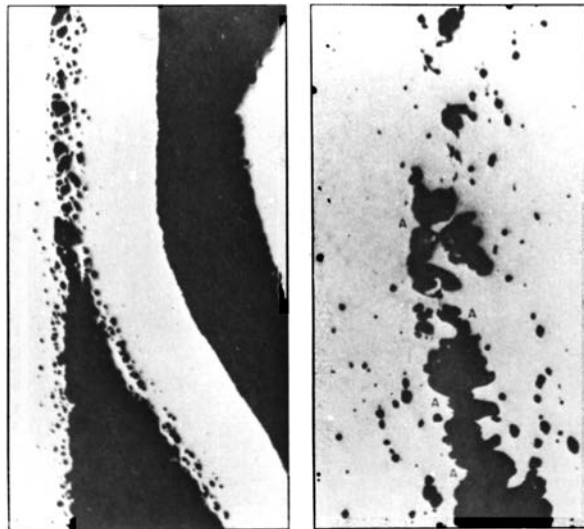


FIG. 14. A sample of full separation of an aluminum target. Impact test performed by SEAMAN *et al.* [107].

Spalling by ductile void formation in nickel is characterized by ellipsoidal cracks with large axes perpendicular to the direction of the applied tensile stress, cf. Fig. 15. A more advanced microdamage process has been shown in Fig. 16, where crack nucleation growth, and coalescence mechanisms in nickel have been observed.

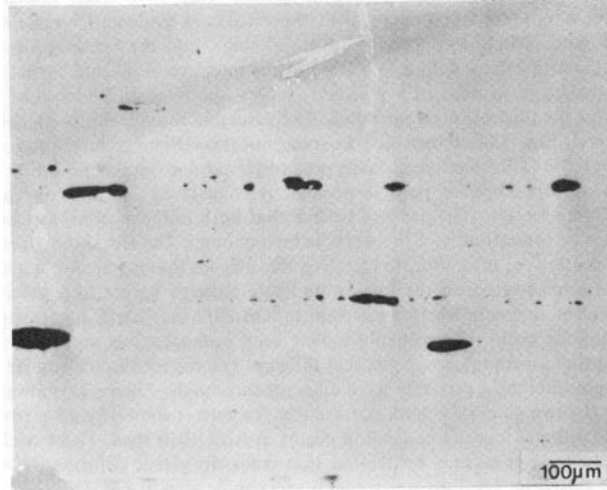


FIG. 15. Spalling by ductile void formation in nickel (After SHOCKEY *et al.* [111]).

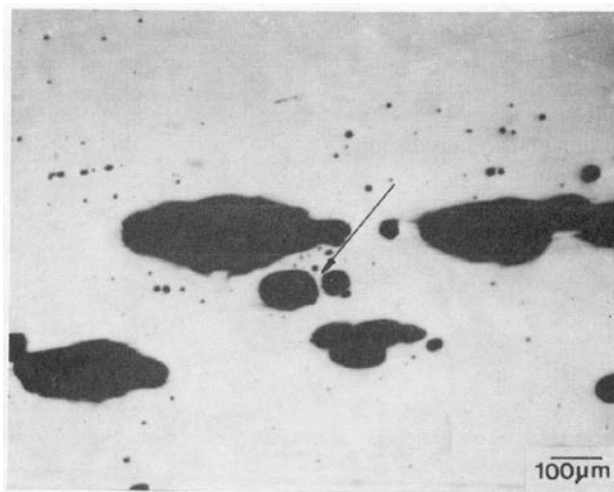


FIG. 16. Void nucleation, growth, and coalescence observed in nickel (After SHOCKEY *et al.* [111]).

Spalling by brittle fracture in low-carbon steel is shown in Fig. 17 (cf. CURRAN *et al.* [24]).



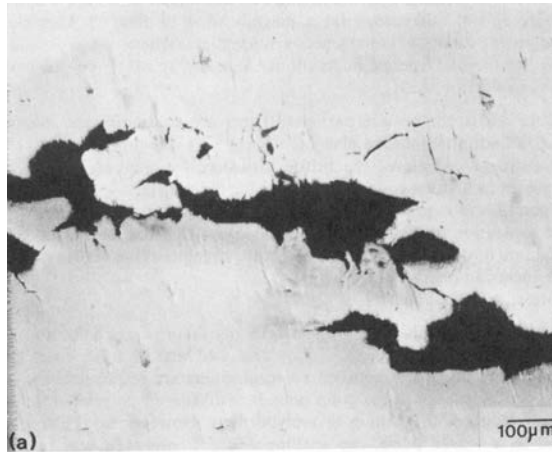


FIG. 17. Spalling by brittle fracture in low-carbon steel (After SHOCKEY *et al.* [111]).

An example of brittle fracture for Armco iron is presented in Fig. 18 (cf. CURRAN *et al.* [24]). It shows the polished cross section through plate impact specimen with very well visible cleavage (penny shape) microcracks. The damage, which appears as randomly oriented planar microcracks, depends on the impact velocity as well as on the duration of the tensile wave. The second property is directly observed from the results presented in Fig. 19 (cf. CURRAN *et al.* [23]). Use of a tapered flyer results in longer tensile impulses at the thicker end. As it is shown in Fig. 19 these longer pulses lead to greater damage in the Armco iron target (the inset gives to approximate durations of the tensile pulses). The damage observed in this experiment is termed brittle, although the microcrack growth is much slower than elastic crack velocities, indicating considerable plastic flow at micro crack tips.

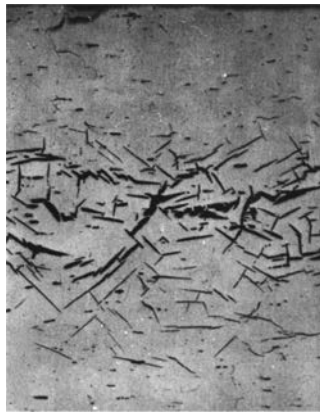


FIG. 18. Internal cleavage (penny shape) microcracks caused by shock loading in the polished cross section of an Armco iron specimen (After CURRAN *et al.* [24]).

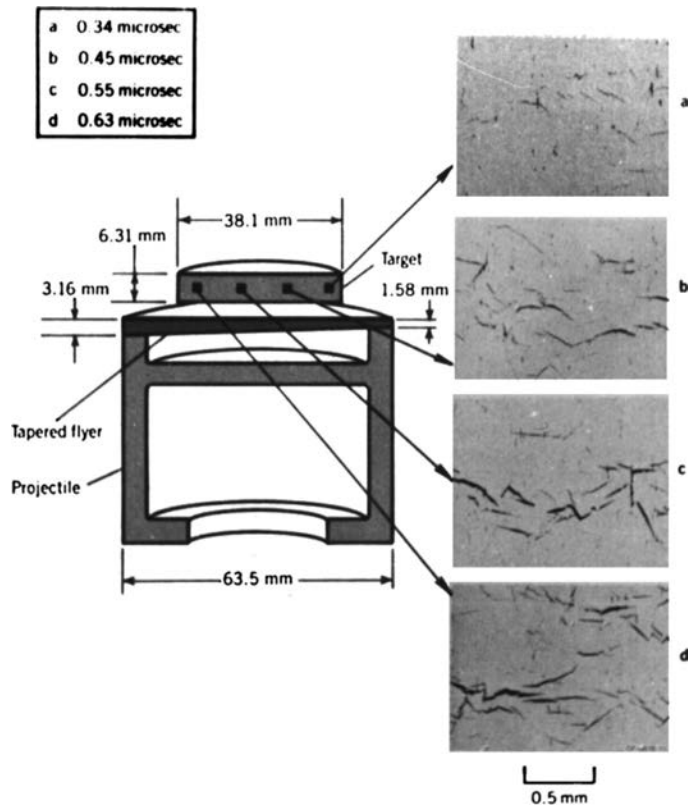


FIG. 19. Tapered flyer impact experimental results for the Armco iron target (After CURRAN *et al.* [23]).

Adiabatic shear band localization during dynamic process can be another good example of anisotropic effects. Shear band form in one direction, which is determined by the state of stress and the properties of the material of a body, as well as by the boundary conditions.

GREBE, PAK and MEYERS [45] were conducted ballistic impact experiments on 12.5 mm thick commercial purity titanium and T-6pct Al-4pct V alloy plates using steel projectiles with 10.5 mm diameter. The impact velocities in their experiments varied between 578 m/s and 846 m/s. The microstructural damage mechanisms associated with shear band formation, shock wave and dynamic fracture were investigated by optical and scanning and transmission electron microscopy. The shear band were found along the two sides of the cross-section passing through the axis of the projectile. The measured shear band width in T6A14V varied between 1 and 10  $\mu\text{m}$ . Observations of the onset of fracture along the shear band were also conducted. Spherical and ellipsoidal microcracks in T6A14V were found along the bands, Fig. 20. The mechanism of final fail-

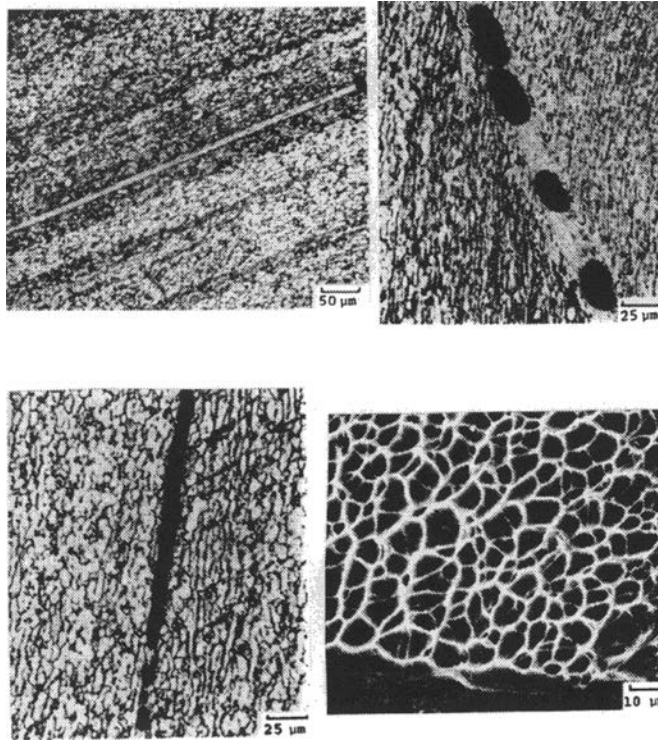


FIG. 20. Shear band in Ti6Al4V target impacted at 846 m/s (After GREBE *et al.* [45]): a) single shear band, b) microcracks in the shear band region, c) elongated macrocracks along the shear band, d) characteristic dimples observed in spall region.

ure in T6A14V is a simple propagation of a macrocrack along the damaged material within the shear band region. In the explanation of the phenomenon of fracture along shear band very important role has the microdamage process which consists of the nucleation, growth and coalescence of microvoids.

The investigations reported by GREBE *et al.* [45] indicated that in dynamic processes the shear band regions behave differently than adjacent zones, cf. Fig. 20. Within the shear band region the deformation process is characterized by very large strains (shear strains over 100%) and very high strain rates ( $10^3$ – $10^5$  s $^{-1}$ ). The strain rate sensitivity of a material becomes very important feature of the shear band region and the micro-damage process is intensified.

*5.1.5. Heuristic multiscale considerations* Let us consider a body  $\mathcal{B}$ , on a part  $\partial\mathcal{B}_1$  of  $\partial\mathcal{B}$  is prescribed sudden deposition of intense pulses of energy, and another part  $\partial\mathcal{B}_2$  is free. This macroscopic situation is shown in Fig. 23 (macroscale). In a body  $\mathcal{B}$  let us consider a subbody  $\mathcal{A}$  with the particle A described by  $(\mathbf{x}, t)$ . Figure 23 (mesoscale) (cf. Fig. 21) shows a typical polished sur-

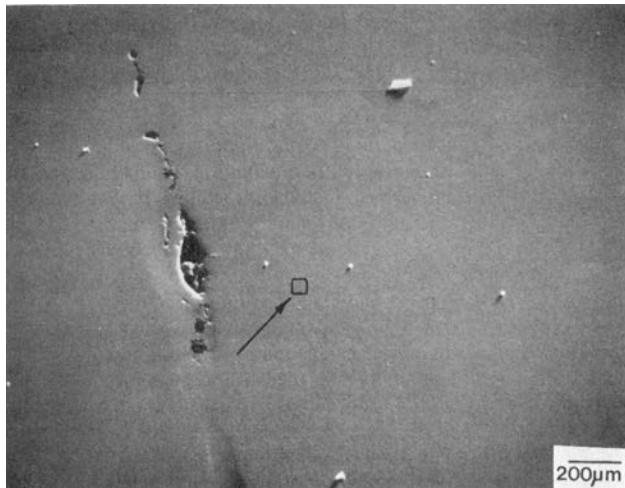


FIG. 21. Appearance of surroundings of spall in nickel (SEM of polished section); square indicates portion that was magnified (After SHOCKEY *et al.* [111]).

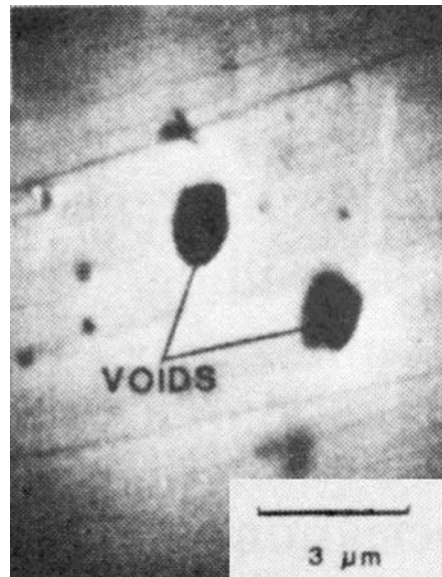


FIG. 22. Magnified view of area shown in Fig. 21; individual photomicrograph taken at 10 000 $\times$  magnification. Two ductile microvoids forming homogeneously in matrix (After SHOCKEY *et al.* [111]).

face of spall nickel, taken from the neighbourhood of a particle A, at a magnification 75 $\times$ . In an attempt to pay attention to smaller microcracks (microvoids), the region marked with a square was observed by scanning-electron microscopy individual photomicrograph is taken at 10 000 $\times$ . Figure 23 (microscale) (cf. Fig. 22)

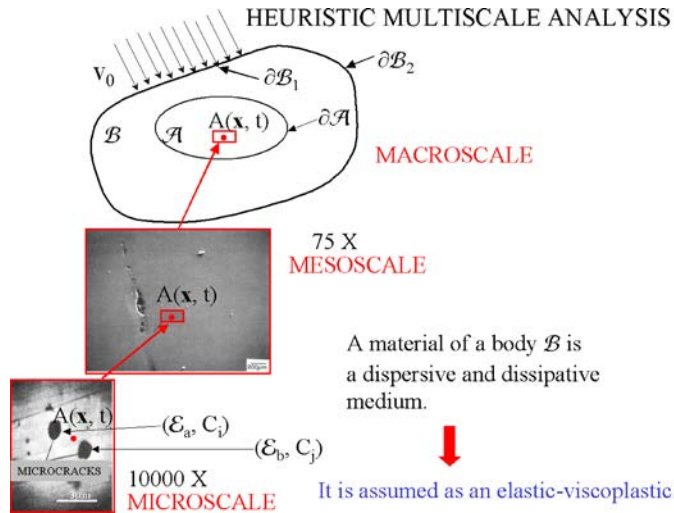


FIG. 23. Heuristic multiscale considerations.

shows two nucleated microcracks in the vicinity of the particle  $A(\mathbf{x}, t)$ . To analyse more precisely the situation in the microscale let us take the properties of nickel into account. We assume that a material of a body  $\mathcal{B}$  is a dispersive and dissipative medium. In a dispersive medium any initial disturbance is broken up into a system of wavegroups. Then the energy is propagated to the particular nucleated microcrack with the group velocity. Thus, each of these two microcracks will receive different portion of energy:  $\varepsilon_a$  and  $\varepsilon_b$ , distributed by the group velocities  $C_i$  and  $C_j$ , respectively. This important fact observed leads to the fundamental conclusion that the evolution of microdamage has anisotropic nature.

As the result of this multiscale analysis we have very crucial suggestions concerning the constitutive description:

(i) Since a material of a body  $\mathcal{B}$  (for various metals like nickel, copper, aluminium, lead and mild steel) is a dispersive and dissipative medium, then it can be modelled as an elastic-viscoplastic.

(ii) Since the dispersive effects for propagation of wave phenomena play so important role, then we have very heterogeneous deformation processes which lead to the residual type stresses and generate the strain induced anisotropy.

(iii) The anisotropy of intrinsic microdamage processes observed experimentally and discussed on the basis of multiscale consideration is very fundamental for the proper description of fracture phenomena.

Finally, we have good foundations to suggest a finite set of the internal state variables. We propose to assume as the internal state variables: the equivalent viscoplastic deformation  $\varepsilon^p$ , which will describe inelastic flow phenomena, the

microdamage second order tensor  $\boldsymbol{\xi}$ , to take account for the anisotropic microdamage mechanisms, and the back stress (residual stress)  $\boldsymbol{\alpha}$ , which will model the kinematic hardening intrinsic mechanism as an approximate description of the strain induced anisotropy.

### 5.2. Constitutive postulates and fundamental assumptions

Our main objective is the development of an elasto-viscoplastic material model within the thermodynamical covariant unique constitutive structure with a finite set of the internal state variables.

Let us assume that we have the material structure with a finite set of the internal state variables  $(\mathcal{G}, \Pi, \Sigma, \widehat{\mathbf{S}}, \widehat{\mathbf{e}})$  and additionally let us introduce for our practical purposes the fundamental postulates as follows:

(i) The internal state variable vector has the form

$$(5.7) \quad m = \boldsymbol{\mu} = (\epsilon^p, \boldsymbol{\xi}, \boldsymbol{\alpha}),$$

thus it consists of one scalar value and two second order tensors, namely the equivalent viscoplastic deformation, i.e.

$$(5.8) \quad \epsilon^p = \int_0^t \left( \frac{2}{3} \mathbf{d}^p; \mathbf{d}^p \right)^{1/2} dt,$$

which aims to describe dissipation generated by elastic-viscoplastic flow phenomena;  $\boldsymbol{\xi}$  denotes the microdamage second order tensor, with the physical interpretation that  $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi$  defines the volume fraction porosity and takes account for dissipation produced by microdamage mechanisms; and  $\boldsymbol{\alpha}$  is the residual stress (the back stress) and aims at the description of dissipation occurred during the kinematic hardening mechanism.

(ii) It is assumed that the free energy function is given by

$$(5.9) \quad \psi = \widehat{\psi}(\mathbf{e}, \mathbf{F}, \vartheta, \boldsymbol{\mu}).$$

(iii) The viscoplastic potential function is defined as

$$(5.10) \quad f = f(\widetilde{J}_1, \widetilde{J}_2, \vartheta, \boldsymbol{\mu}),$$

where  $\widetilde{J}_1, \widetilde{J}_2$  denote the first two invariants of the stress tensor  $\widetilde{\boldsymbol{\tau}} = \boldsymbol{\tau} - \boldsymbol{\alpha}$ .

(iv) It is proposed the evolution equations for a set of the internal state variables

$$(5.11) \quad \mathbf{d}^p = \Lambda \mathbf{P}, \quad \mathbf{L}_v \boldsymbol{\xi} = \boldsymbol{\Xi}, \quad \mathbf{L}_v \boldsymbol{\alpha} = \mathbf{A}$$

and for the plastic spin

$$(5.12) \quad \boldsymbol{\omega}^p = \Lambda \boldsymbol{\Omega},$$

where for an elasto-viscoplastic model of a material we assume (cf. PERZYNA [70, 71, 72, 73, 87, 88, 91])

$$(5.13) \quad \Lambda = \frac{1}{T_m} \left\langle \Phi \left( \frac{f}{\kappa} - 1 \right) \right\rangle,$$

$T_m$  denotes the relaxation time for mechanical disturbances, the isotropic work-hardening-softening function is

$$(5.14) \quad \kappa = \widehat{\kappa}(\boldsymbol{\epsilon}^p, \vartheta, \boldsymbol{\xi}),$$

$\Phi$  is the empirical overstress function, the bracket  $\langle \cdot \rangle$  defines the ramp function,

$$(5.15) \quad \mathbf{P} = \frac{\partial f}{\partial \boldsymbol{\tau}} \Big|_{\boldsymbol{\xi}=\text{const}} \left( \left\| \frac{\partial f}{\partial \boldsymbol{\tau}} \right\| \right)^{-1},$$

$\boldsymbol{\Xi}$ ,  $\mathbf{A}$  and  $\boldsymbol{\Omega}$  denote the evolution functions which have to be determined.

### 5.3. Microshear banding effects

To describe the microshear banding effects let us assume that the relaxation time  $T_m$  depends on the active microshear bands fraction  $f_{ms}$  and on the rate of equivalent viscoplastic deformation  $\dot{\boldsymbol{\epsilon}}^P$  (cf. PEŁCERSKI [100], NOWAK *et al.* [67], Perzyna [92]), i.e.

$$(5.16) \quad T_m = T_m(f_{ms}, \dot{\boldsymbol{\epsilon}}^P).$$

Additionally we introduce the simplification as follows

$$(5.17) \quad T_m = T_m^0 \phi_1(f_{ms}) \phi_2(\dot{\boldsymbol{\epsilon}}^P).$$

For example, for mild steel (cf. Perzyna [92]) we can postulate

$$(5.18) \quad \phi_1(f_{ms}) = [1 - f_{ms}(\boldsymbol{\epsilon}^P)] = \left[ 1 - f_{ms}^0 \frac{1}{1 + \exp(a - b \boldsymbol{\epsilon}^P)} \right],$$

and

$$(5.19) \quad \phi_2(\dot{\boldsymbol{\epsilon}}^P) = \left( \frac{\dot{\boldsymbol{\epsilon}}^P}{\dot{\boldsymbol{\epsilon}}_s^P} - 1 \right)^{1/p},$$

where  $f_{ms}^0$ ,  $a$ ,  $b$  and  $p$  are material parameters.

Finally we have

$$(5.20) \quad T_m = T_m^0 \left[ 1 - f_{ms}^0 \frac{1}{1 + \exp(a - b \boldsymbol{\epsilon}^P)} \right] \left( \frac{\dot{\boldsymbol{\epsilon}}^P}{\dot{\boldsymbol{\epsilon}}_s^P} - 1 \right)^{1/p}.$$

#### 5.4. Constitutive assumption for the plastic spin

Let us postulate that  $\mathbf{\Omega}$  has the form<sup>20)</sup> (cf. DAFALIAS [26] and LORET [57])

$$(5.21) \quad \mathbf{\Omega} = \eta^*(\boldsymbol{\alpha} \cdot \mathbf{P} - \mathbf{P} \cdot \boldsymbol{\alpha}),$$

where  $\eta^*$  denotes the scalar valued function of the invariants of the tensors  $\boldsymbol{\alpha}$ ,  $\boldsymbol{\xi}$  and  $\mathbf{P}$ , and may depend on temperature  $\vartheta$ .

#### 5.5. Anisotropic intrinsic microdamage mechanisms

To take into consideration the observed time dependent effects it is advantageous to use the proposition of the description of the intrinsic microdamage process presented by PERZYNA [83, 84], DUSZEK-PERZYNA, PERZYNA [32], and DORNOWSKI, PERZYNA [28].

Let us assume that the intrinsic microdamage process consists of the nucleation and growth mechanisms<sup>21)</sup>.

Based on the heuristic suggestions and taking into account the influence of the stress triaxiality and anisotropic effects on the nucleation and growth mechanisms we assume the evolution equation for the microdamage tensor  $\boldsymbol{\xi}$  as follows

$$(5.22) \quad \mathbf{L}\boldsymbol{\nu}\boldsymbol{\xi} = \frac{\partial h^*}{\partial \boldsymbol{\tau}} \frac{1}{T_m} \left\langle \Phi \left[ \frac{\tilde{I}_n}{\tau_n(\boldsymbol{\xi}, \boldsymbol{\alpha}, \vartheta, \epsilon^p)} - 1 \right] \right\rangle + \frac{\partial g^*}{\partial \boldsymbol{\tau}} \frac{1}{T_m} \left\langle \Phi \left[ \frac{\tilde{I}_g}{\tau_{eq}(\boldsymbol{\xi}, \boldsymbol{\alpha}, \vartheta, \epsilon^p)} - 1 \right] \right\rangle.$$

The tensorial function  $\frac{\partial h^*}{\partial \boldsymbol{\tau}}$  describes the mutual microcrack interaction for nucleation mechanism, while the tensorial function  $\frac{\partial g^*}{\partial \boldsymbol{\tau}}$  represents the mutual microcrack interaction for growth process,  $\tau_n$  and  $\tau_{eq}$  denote the threshold stresses for microcrack nucleation and growth, respectively.

$$(5.23) \quad \tilde{I}_n = a_1 \tilde{J}_1 + a_2 \sqrt{\tilde{J}_2} + a_3 (\tilde{J}_3)^{1/3}$$

<sup>20)</sup>For a thorough discussion of a concept of the plastic spin and its constitutive description in phenomenological theories for macroscopic large plastic deformations please consult the critical review paper by VAN DER GIESSEN [117].

<sup>21)</sup>Recent experimental observation results (cf. SHOCKEY *et al.* [112]) have shown that coalescence mechanism can be treated as nucleation and growth process on a smaller scale.



defines the stress intensity invariant for nucleation,  $a_i$  ( $i = 1, 2, 3$ ) are the material constants,  $\tilde{J}'_2$  and  $\tilde{J}'_3$  are the second and third invariants of the stress deviator  $\tilde{\boldsymbol{\tau}}' = (\boldsymbol{\tau} - \boldsymbol{\alpha})'$ ,

$$(5.24) \quad \tilde{I}_g = b_1 \tilde{J}_1 + b_2 \sqrt{\tilde{J}'_2} + b_3 \left( \tilde{J}'_3 \right)^{1/3},$$

defines the stress intensity invariant for growth and  $b_i$  ( $i = 1, 2, 3$ ) are the material constants. This determines the evolution function  $\Xi$ .

In the evolution equation (5.22) the functions

$$(5.25) \quad h = \hat{h}(\boldsymbol{\tau}, \vartheta, \in^P, \boldsymbol{\xi}, \boldsymbol{\alpha}),$$

$$(5.26) \quad g = \hat{g}(\boldsymbol{\tau}, \vartheta, \in^P, \boldsymbol{\xi}, \boldsymbol{\alpha})$$

play the fundamental role, and have to be determined based on available experimental observation data. We also introduced the denotations as follows

$$(5.27) \quad \frac{\partial h^*}{\partial \boldsymbol{\tau}} = \frac{\partial \hat{h}}{\partial \boldsymbol{\tau}} \left( \left\| \frac{\partial \hat{h}}{\partial \boldsymbol{\tau}} \right\| \right)^{-1}, \quad \frac{\partial g^*}{\partial \boldsymbol{\tau}} = \frac{\partial \hat{g}}{\partial \boldsymbol{\tau}} \left( \left\| \frac{\partial \hat{g}}{\partial \boldsymbol{\tau}} \right\| \right)^{-1}.$$

The threshold stress  $\tau_n$  and  $\tau_{eq}$  for microcrack nucleation and growth, respectively, can be assumed as the material functions in the form

$$(5.28) \quad \tau_n = \tau_n(\boldsymbol{\xi}, \boldsymbol{\alpha}, \vartheta, \in^P), \quad \tau_{eq} = \tau_{eq}(\boldsymbol{\xi}, \boldsymbol{\alpha}, \vartheta, \in^P).$$

### 5.6. Kinematic hardening

To determine the evolution function  $\mathbf{A}$  we shall follow some results obtained by DUSZEK, PERZYNA [30]. The kinematic hardening evolution law takes the form

$$(5.29) \quad \mathbf{L}_v \boldsymbol{\alpha} = \frac{1}{T_m} \left\langle \Phi \left( \frac{f}{\kappa} - 1 \right) \right\rangle \left[ r_1 \mathbf{P} + r_2 \frac{\mathbf{P} : \mathbf{Q}}{\tilde{\boldsymbol{\tau}} : \mathbf{Q} + r_3 \boldsymbol{\xi} : \mathbf{Q}} (\tilde{\boldsymbol{\tau}} + r_3 \boldsymbol{\xi}) \right],$$

where  $r_1$ ,  $r_2$  and  $r_3$  are the material coefficients and

$$(5.30) \quad \mathbf{Q} = \left[ \frac{\partial f}{\partial \boldsymbol{\tau}} + \left( \frac{\partial f}{\partial \boldsymbol{\xi}} - \frac{\partial \kappa}{\partial \boldsymbol{\xi}} \right) : \frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{\tau}} \right] \left\| \frac{\partial f}{\partial \boldsymbol{\tau}} + \left( \frac{\partial f}{\partial \boldsymbol{\xi}} - \frac{\partial \kappa}{\partial \boldsymbol{\xi}} \right) : \frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{\tau}} \right\|^{-1}.$$

The kinetic law (5.29) represents the linear combination of the Prager and Ziegler kinematic hardening rules and additionally depends linearly on the microdamage tensor  $\boldsymbol{\xi}$ .

5.7. *Thermodynamic restrictions and rate type constitutive relations*

Suppose the axiom of the entropy production holds. Then the constitutive assumption (5.9) and the evolution equations (5.11) and (5.12) lead to the results as follows

$$(5.31) \quad \boldsymbol{\tau} = \rho_{Ref} \frac{\partial \hat{\psi}}{\partial \mathbf{e}}, \quad \eta = -\frac{\partial \hat{\psi}}{\partial \vartheta}, \quad -\frac{\partial \hat{\psi}}{\partial \boldsymbol{\mu}} \cdot \mathbf{L}\boldsymbol{\nu}\boldsymbol{\mu} - \frac{1}{\rho\vartheta} \mathbf{q} \cdot \text{grad}\vartheta \geq 0.$$

The rate of internal dissipation is determined by

$$(5.32) \quad \vartheta \hat{i} = -\frac{\partial \hat{\psi}}{\partial \boldsymbol{\mu}} \cdot \mathbf{L}\boldsymbol{\nu}\boldsymbol{\mu} \\ = -\left[ \frac{\partial \hat{\psi}}{\partial \epsilon^P} \sqrt{\frac{2}{3}} + \frac{\partial \hat{\psi}}{\partial \boldsymbol{\alpha}} : \left( r_1 \mathbf{P} + r_2 \frac{\mathbf{P} : \mathbf{Q}}{\tilde{\boldsymbol{\tau}} : \mathbf{Q} + r_3 \boldsymbol{\xi} : \mathbf{Q}} (\tilde{\boldsymbol{\tau}} + r_3 \boldsymbol{\xi}) \right) \right] \Lambda - \frac{\partial \hat{\psi}}{\partial \boldsymbol{\xi}} : \boldsymbol{\Xi}.$$

Operating on the stress relation (5.31)<sub>1</sub> with the Lie derivative and keeping the internal state vector constant, we obtain

$$(5.33) \quad \mathbf{L}\boldsymbol{\nu}\boldsymbol{\tau} = \mathcal{L}^e : \mathbf{d} - \mathcal{L}^{th} \dot{\vartheta} - [(\mathcal{L}^e + \mathbf{g}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{g} + \boldsymbol{\gamma}\mathcal{W}) : \mathbf{P}] \frac{1}{T_m} \left\langle \Phi \left( \frac{f}{\kappa} - 1 \right) \right\rangle,$$

where

$$(5.34) \quad \mathcal{L}^e = \rho_{Ref} \frac{\partial^2 \hat{\psi}}{\partial \mathbf{e}^2}, \quad \mathcal{L}^{th} = -\rho_{Ref} \frac{\partial^2 \hat{\psi}}{\partial \mathbf{e} \partial \vartheta}, \\ \boldsymbol{\gamma}\mathcal{W} = \eta^* [(\mathbf{g}\boldsymbol{\tau} - \boldsymbol{\tau}\mathbf{g}) : (\boldsymbol{\alpha}\mathbf{g} - \mathbf{g}\boldsymbol{\alpha})].$$

Substituting  $\dot{\psi}$  into the energy balance equation (3.5) and taking into account the results (5.31)<sub>3</sub> and (5.32) gives

$$(5.35) \quad \rho\vartheta \dot{\eta} = -\text{div}\mathbf{q} + \rho\vartheta \hat{i}.$$

Operating on the entropy relation (5.31)<sub>2</sub> with the Lie derivative and substituting the result into (5.35) we obtain

$$(5.36) \quad \rho c_p \dot{\vartheta} = -\text{div}\mathbf{q} + \vartheta \frac{\rho}{\rho_{Ref}} \frac{\partial \boldsymbol{\tau}}{\partial \vartheta} : \mathbf{d} + \rho \chi^* \boldsymbol{\tau} : \mathbf{d}^p + \rho \chi^{**} \mathbf{K} : \mathbf{L}\boldsymbol{\nu}\boldsymbol{\xi},$$

where the specific heat

$$(5.37) \quad c_p = -\vartheta \frac{\partial^2 \hat{\psi}}{\partial \vartheta^2},$$

and the irreversibility coefficients  $\chi^*$  and  $\chi^{**}$  are determined by

$$(5.38) \quad \begin{aligned} \chi^* = & - \left[ \left( \frac{\partial \widehat{\psi}}{\partial \in^P} - \vartheta \frac{\partial^2 \widehat{\psi}}{\partial \vartheta \partial \in^P} \right) \sqrt{\frac{2}{3}} + \left( \frac{\partial \widehat{\psi}}{\partial \alpha} - \vartheta \frac{\partial^2 \widehat{\psi}}{\partial \vartheta \partial \alpha} \right) \right. \\ & \left. : \left( r_1 \mathbf{P} + r_2 \frac{\mathbf{P} : \mathbf{Q}}{\widehat{\tau} : \mathbf{Q} + r_3 \boldsymbol{\xi} : \mathbf{Q}} (\widehat{\tau} + r_3 \boldsymbol{\xi}) \right) \right] \frac{1}{\tau : \mathbf{P}}, \\ \chi^{**} \mathbf{K} = & - \left( \frac{\partial \widehat{\psi}}{\partial \boldsymbol{\xi}} - \vartheta \frac{\partial^2 \widehat{\psi}}{\partial \vartheta \partial \boldsymbol{\xi}} \right). \end{aligned}$$

### 5.8. Fracture criterion based on the evolution of microdamage

We base the fracture criterion on the evolution of the microdamage tensor  $\boldsymbol{\xi}$ .

Let us assume that for  $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi^F$  catastrophe takes place (cf. PERZYNA [82]), that is

$$(5.39) \quad \kappa = \widehat{\kappa}(\in^P, \vartheta, \boldsymbol{\xi})|_{(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi^F} = 0.$$

It means that for  $(\boldsymbol{\xi} : \boldsymbol{\xi})^{1/2} = \xi^F$  the material loses its carrying capacity. The condition (5.39) describes the main feature observed experimentally that the load tends to zero at the fracture point.

It is noteworthy that the isotropic hardening-softening material function  $\widehat{\kappa}$  proposed in Eq. (5.14) should satisfy the fracture criterion (5.39).

### 5.9. Length-scale sensitivity of the constitutive model

The constitutive equations for a thermo-elastic-viscoplastic model introduce implicitly a length-scale parameter into the dynamic initial-boundary value problem, i.e.

$$(5.40) \quad l = \beta c T_m \quad \text{or} \quad l = \beta c T_m^0 \phi_1(f_{ms}) \phi_2(\dot{\in}^P),$$

and as example for mild steel we have

$$(5.41) \quad l = \beta c T_m^0 \left[ 1 - f_{ms}^0 \frac{1}{1 + \exp(a - b \in^P)} \right] \left( \frac{\dot{\in}^P}{\dot{\in}_s^P} - 1 \right)^{1/p},$$

where  $T_m$  is the relaxation time for mechanical disturbances, and is directly related to the viscosity of the material,  $c$  denotes the velocity of the propagation of the elastic waves in the problem under consideration, and the proportionality factor  $\beta$  depends on the particular initial-boundary value problem and may also be conditioned on the microscopic properties of the material.

The relaxation time  $T_m$  can be viewed either as a microstructural parameter to be determined from experimental observations or as a mathematical regularization parameter.

It is noteworthy to stress that the length-scale sensitivity of the constitutive structure is of great importance for proper description of meso- and micromechanical problems.

## 6. EPILOGUE

Our description of the thermo-elasto-viscoplastic constitutive structure is invariant with respect to any diffeomorphism. It means that the constitutive structure is invariant to any superposed motion<sup>22)</sup>. Such constitutive structure is called covariant, cf. MARS DEN, HUGHES [58].

The covariance property of the constitutive structure has been achieved due to the assumption that the rates of the deformation tensors and the stress tensors (as well as all vectors and tensors) are defined based on the Lie derivative. Of course, the covariance description has very important consequence for proper mathematical investigations of some phenomena which can be discussed in the solution of the evolution problems. It will be also very crucial for proper description of meso-, micro-, and nano-mechanical problems and particularly in their numerical solutions.

The experimental works have brought deep understanding of the evolution of the dislocation substructure and the intrinsic microdamage mechanism during dynamic loading processes and clearly have shown that microshear banding influence a substructure of a polycrystalline material and fracture mechanism of metals does very much depend on the strain rate and wave shape effects.

The crucial idea in the theory of elasto-viscoplasticity developed is the very efficient interpretation of a finite set of the internal state variables as the equivalent plastic deformation, the microdamage tensor and the residual stress (the back stress). To describe suitably the time and temperature dependent effects observed experimentally and the accumulation of the plastic deformation and anisotropic damage during dynamic loading processes the thermomechanical coupling has been taken into account and the kinetics of microdamage and kinematic hardening law have been modified and generalized.

It is very well known fact that the stress wave propagation in an elasto-viscoplastic medium has the dispersive nature.

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<sup>22)</sup>We can say that the thermodynamical theory of elasto-viscoplasticity satisfies very crucial property of symmetry, because is invariant with respect to diffeomorphism transformation, it means, that it is symmetric with respect to arbitrary motion, cf. NOETHER [63], LEDERMAN, HILL [55] and PENROSE [69].

**The dispersion effect** is very important for the development of the regularization procedure for the rate independent plastic flow evolution problems.

The dispersion effect is very crucial for the proper description of induced anisotropy. In the dynamical problems in solids, the dispersive wave phenomena are generated the induced anisotropy of two different kinds. First, is generated by the residual stresses which result from very heterogeneous deformation process. Second, is caused by intrinsic microdamage mechanism, is observed experimentally and suggested by multiscale considerations. Both kinds of the induced anisotropy influence very much the development of fracture phenomena in solids.

Of course, the dispersion effects will also influence very much the initiation and development of localization phenomena. A thorough analysis of these consequences has been presented in GLEMA *et al.* [41, 42, 43].

Very recently, it has been widely recognized to consider an elastic-viscoplastic model of a material as a regularization method for solving mesh-dependent problems of plasticity. In these regularized initial-boundary value problems, wave propagation phenomena play a fundamental role. An elastic-viscoplastic model introduces dissipative as well as dispersive nature for the propagated waves. The dispersion property implies that in the elastic-viscoplastic medium any initial disturbance can break up into a system of group of oscillations or wavelets. On the other hand, the dissipation property causes the amplitude of a harmonic wavetrain to decay with time. In the evolution problem considered in such dissipative and dispersive medium, the stress deformation due to wave reflections and interactions are not uniformly distributed, and this kind of heterogeneity can lead to strain localization in the absence of geometrical or material imperfections.

Since the rate independent plastic response is obtained as the limit case when the relaxation time is equal to zero hence the theory of elasto-viscoplasticity offers the regularization procedure for the solution of the dynamical initial-boundary value problems. The viscoplastic regularization procedure assures the stable integration algorithm by using the finite difference or finite element methods.

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