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Modelling adiabatic shear banding via damage mechanics approach

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Dedicated to Professor Piotr Perzyna on the occasion of his 70^{th} birthday

DURING DYNAMIC LOADING PROCESSES, large plastic deformation associated with high strain rates leads, for a broad class of ductile metals, to degradation and failure by adiabatic shear banding. The paper presents an attempt to model some salient features of this process viewed as an anisotropic damage mechanism coupled with thermo-elastic/viscoplastic deformation. The model is destined to be applied in the context of high velocity impact and penetration mechanics. The methodology employed within the framework of the internal state variable structure strives to keep a middle way between extensive description of complex viscoplastic flow and damage events and application-oriented accessibility requirements. Model capabilities are prelaminarily illustrated for shear loading process.

1. Introduction and scope

DYNAMIC LOADING CONDITIONS such like high-velocity impact and penetration (see Figs. 1, 2), explosive vs. metal interaction, high-speed machining and other, imply high strain-rate viscoplastic flow characterized by negligible redistribution of the heat generated by plastic deformation. The process is essentially adiabatic and leads to thermal softening which, at some advanced stage of deformation, becomes prevailing against the strain and strain-rate hardening. One observes a decrease in the flow stress and large plastic strain localization within narrow regions known as adiabatic shear bands. The latter are most frequently

observed in high-strength alloys and steels (see e.g. WOODWARD [1] and NEMAT-NASSER *et al.* [2]). A significant temperature difference exists between the inside of bands and the outside. Adiabatic shear band localization phenomena are generally attributed to plastic instability events generated by thermal softening, see e.g. BAI [3] and WRIGHT and BATRA [4]. Extensive investigation and literature have been devoted to the matter in the 1980's and later. The experimental studies by MARCHAND and DUFFY [5], employing thin-walled tubes twisted at high strain rates by means of a torsional KOLSKY bar set-up, are most frequently cited. The reader can find more references, including the earliest investigations into the fracturing by adiabatic shear banding from the mid of the 20^{th} century on, in WOODWARD [1]. As stated by MERCIER and MOLINARI [6], most of the early theoretical approaches to the subject considered a shear band as a one-dimensional entity in a much simplified context of material behaviour. A great number of studies in the 1990's went deeper into multiform material parameter influence on multiple shear band forming, spacing, characteristic thickness and related propagation phenomena (velocity, extension of the process zone), see e.g. MOLINARI [7] and GRADY [8]. Most of those analyses are performed by zooming on an elementary layer under simple shear loading conditions. Various approaches of instability have been advanced and connected with the geometric pattern of shear bands, e.g. MOLINARI [7] and PĘCHERSKI [9].

PERZYNA was probably the first to have incorporated the shear band formation into three-dimensional (3D) modelling, regarding viscoplastic flow coupled with micro-damage process embodied by specific internal variable(s). In the paper [10] adiabatic shear band localization under dynamic loading conditions has been considered together with spalling by ductile void formation in the modelling framework insisting on and turned towards induced anisotropic effects. The microdamage mechanism by nucleation and growth of microcracks is dealt with in [10]. The anisotropic nature of the process is accounted for by specific hypotheses concerning the distribution and the shape of defects including a random nature of micro-damage evolution. The more recent papers by ŁODYGOWSKI and PERZYNA [11] and DORNOWSKI and PERZYNA [12] focus even more on fracturing phenomena related to localized adiabatic shearing in a quantitatively elaborated damage modelling coupled with thermo-viscoplastic flow. The well-posedness of the evolution problem and numerical regularization aspects are discussed in the framework of consistent formulation of the discretized initial-boundary-value problem.

The objectives of the present paper are clearly situated in the above perspective traced by PERZYNA's damage-and-viscoplasticity 3D modelling of ductile metals at large strains and high strain rates. Including specific anisotropy effects induced by a particular deterioration mechanism, i.e. shear banding related damage, it is being done in an alternative manner based on the second

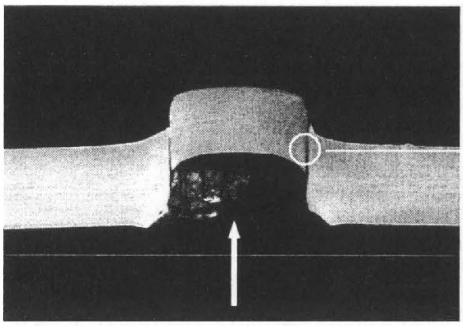

FIG. 1. Impacted hard steel plate (after GIAT Industries).

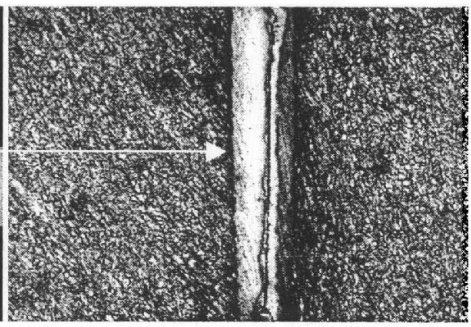

FIG. 2. Adiabatic shear band with ultimate crack (after GIAT Industries).

authors earlier contributions to anisotropic damage, see e.g. the synthetic review by DRAGON *et al.* [13]. The highly non-trivial and still arduous problem of combining finite-strain plasticity and anisotropy effects is being considered here using Mandel-Sidoroff framework, see e.g. MANDEL [14] and SIDOROFF and DOGUI [15].

The present work presents an attempt to model some salient features of damage by shear banding as coupled with thermo-elastic/viscoplastic deformation, involving multifold anisotropy effects while introducing some simplifying hypotheses (e.g. as concerns plastic hardening). The purpose is to get a tractable model to be applied in the context of high-velocity impact and penetration mechanics.

The paper is organized as follows: in Sec. 2 preliminary remarks concerning internal damage variable related to adiabatic shear bands (ASB) are given and some terminology is introduced. In Sec. 3 large deformation thermo-elastic/viscoplastic model with internal variables and damage-induced anisotropy effects is introduced and discussed. An auxiliary analysis, allowing for evaluation of the onset of instability via thermo-viscoplastic perturbation method, is employed to pose a damage-inception criterion. This analysis is summarized in Sec. 4. In Sec. 5 the constitutive model is preliminarily but extensively tested on a homogeneous volume element (material point) under simple shear loading. Some comments concerning the identification and bounding of material parameters are also given in Sec. 5.

2. The ASB-related damage variable and kinematic preliminaries

In this paper, we are interested in the description of the material behaviour in the presence of ASB considered as damage mechanism to be put forward in the framework of a 3D continuous model: within this model, the deterioration

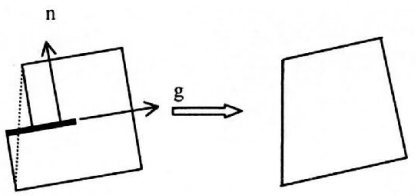

FIG. 3. Equivalent homogeneous volume element ($\alpha = 1$).

at stake is to be captured by a corresponding internal variable, its evolution and its effect on elastic stiffness and viscoplastic flow. The model should be robust enough to overcome local instabilities relative to inception and growth of ASB on mesoscale level. Another feature to be accounted for by this model is a strongly oriented character of ASB, thus inducing significant mechanical anisotropy with both elasticity and plasticity being potentially affected.

In order to describe the anisotropic degradation state of the material caused by the presence of ASB, a 2nd order tensorial damage variable is introduced. Its components are denoted as D_{ij} and are expressed by (2.1), where d^α and $\mathbf{n}^\alpha$ represent respectively the scalar intensity and the orientation of the band pattern α (see Fig. 3).

$$
\begin{aligned}
D_{ij} &= \sum_\alpha d^\alpha \cdot N_{ij}^\alpha , \\
N_{ij}^\alpha &= n_i^\alpha n_j^\alpha .
\end{aligned}
\tag{2.1}
$$

As discussed before, the onset and further evolution of adiabatic shear banding are a consequence of thermal softening, respectively in the sound material during locally homogeneous plastic deformation, and inside the bands themselves during evolving localization process. The intensity d^α includes consequently information relative to temperature inside the band pattern α. Consider now a single band pattern ($\alpha = 1$), and introduce the adjective "singular" for the processes relevant strictly to the adiabatic shear banding, and the adjective "regular" for the processes not relevant to the adiabatic shear banding. With such a distinction, the current density d of the damage variable $\mathbf{D}$ depends on "singular" temperature, and can thus be written as:

$$
d = d(T^*, ...) \tag{2.2}
$$

where T^* represents the "singular" temperature, and where the dots represent other possible arguments.

The lower bound $d_{\min} = d(T_0^*, ...)$ of the density d is obviously zero, T_0^* representing the initial "singular" temperature value which is equal to the "regular"

temperature value at the incipience of damage. On the other hand, temperature is supposed to be bounded in the band material by the melting point. This is probably a strongly over-estimating statement (see e.g. [1]) for metallic materials subject to this mechanism of adiabatic shear banding. The density d of the damage variable $\mathbf{D}$ is consequently bounded too. The upper bound of d is denoted by $d_{\max} = d(T_m, ...)$, where T_m represents the temperature value at the melting point. In Sec. 5, an estimation of $d_{\max}$ is given based on mechanical considerations for the case of simple shear.

The geometric consequences of the shear band pattern (Fig. 3) are viewed as those of a "super-dislocation" (see also PĘCHERSKI [9]). By using concepts of the crystalline plasticity, the damage-induced supplementary strain rate $\mathbf{d^d}$ is introduced as the result of the glide velocity $\dot{\gamma}^\alpha$ caused by the band pattern α of normal $\mathbf{n^\alpha}$ and with orientation $\mathbf{g^\alpha}$ (see Fig. 3):

$$
\begin{aligned}
d_{ij}^d &\propto \sum_\alpha \dot{\gamma}^\alpha M_{ij}^\alpha, \\
M_{ij}^\alpha &= \left(g_i^\alpha n_j^\alpha\right)^S = \frac{1}{2}\left(g_i^\alpha n_j^\alpha + g_j^\alpha n_i^\alpha\right).
\end{aligned}
\tag{2.3}
$$

The kinematic variable $\mathbf{d^d}$ allows to smooth the boundary discontinuity caused by the ASB (see Fig. 3). There are thus two contributions to the inelastic evolution of the equivalent homogeneous volume element: the "regular" plastic strain rate, denoted by $\mathbf{d^p}$, and the "singular" damage induced strain rate, denoted by $\mathbf{d^d}$. The total inelastic strain rate $\mathbf{d^{dp}}$ is written as the sum of those two contributions:

$$
d_{ij}^{dp} = d_{ij}^p + d_{ij}^d \,. \tag{2.4}
$$

Further on, care must be taken to ensure the concomitance of the two rates $\overset{0}{\mathbf{D}}$ (an objective derivative of $\mathbf{D}$ to be defined) and $\mathbf{d^d}$, which are both relative to the same process of ASB-induced damage.

On the other hand, very large strains and rotations occurring during the adiabatic shear banding process make the finite elastic-plastic deformation framework indispensable. Since pioneer MANDEL's works [14], many valuable contributions appeared concerning the introduction of (initial and/or induced) anisotropy in the context of large elastic-plastic strains. Despite this, the problem remains still open, see e.g. SIDOROFF and DOGUI [15] and EKH and RUNESSON [16]. In the present approach, a spatial vision of the motion is adopted in order to preserve the physical signification of the state variables, of their derivatives and of their conjugate forces. Clearly, the Eulerian point of view is suitable to deal with plasticity whose rheology is close to the fluid one in some aspects [15]. However, the Eulerian point of view is not proper to identify material symmetries. In isotropic

elastic-plastic media, the rotation required to define the intermediate configuration is in fact of secondary importance, and rotational and material derivatives lead to the objectivity of the incremental constitutive model as well. With regard to anisotropic elastic-plastic media, the definition of the rotation becomes essential [14].

3. Large deformation damage-viscoplasticity constitutive model with ASB-anisotropy effects

The constitutive model to be formulated must be able to describe the thermo-elastic/viscoplastic behaviour of the sound material and the mechanical anisotropy (directional degradation of both the elastic and viscoplastic moduli) induced by ASB. As stated above, the framework of large elastic-plastic deformation with anisotropy is put forward.

3.1. Large elastic-plastic deformation kinematics including anisotropy

Let $\mathcal{C}_0$ be the initial undeformed configuration of the material, and $\mathcal{C}_t$ its deformed configuration at current time t. In order to account for finite elastic-plastic strains — plastic means here inelastic in the sense of both plastic "regular" and damage-induced "singular" terms — the pseudo intermediate configuration $\mathcal{C}_{\text{inter}}$ is introduced by elastic unloading with respect to the current configuration $\mathcal{C}_t$. Because arbitrary local rotations superposed to relaxed state give alternative intermediate configurations, $\mathcal{C}_{\text{inter}}$ is generally non-unique. The deformation gradient $\mathbf{F}$ from $\mathcal{C}_0$ to $\mathcal{C}_t$ is conventionally decomposed as the product $\mathbf{F} = \mathbf{F^e F^{dp}}$ $\left(F_{iJ} = F^e_{i\alpha} F^{dp}_{\alpha J}\right)$, where $\mathbf{F^{dp}}$ denotes the "damage-plastic" transformation from $\mathcal{C}_0$ to $\mathcal{C}_{\text{inter}}$, and $\mathbf{F^e}$ denotes the elastic transformation from $\mathcal{C}_{\text{inter}}$ to $\mathcal{C}_t$.

In the present case, anisotropy is induced by damage (in the form of adiabatic shear bands) during inelastic transformation $\mathbf{F^{dp}}$. It then seems to be natural to define anisotropy in the intermediate configuration $\mathcal{C}_{\text{inter}}$ that becomes henceforth a pseudo-material configuration (see also LUBARDA [17]).

During inelastic deformation $\mathbf{F^{dp}}$, matter is moving with respect to the laboratory fixed frame $\mathcal{S}$. This motion can be decomposed as the sum of the motion of the matter with respect to the anisotropy axes $\mathcal{A}$ and the motion of the anisotropy axes $\mathcal{A}$ with respect to the laboratory frame $\mathcal{S}$. To maintain the axes of anisotropy (damage tensor eigenvectors) $\mathcal{A}$ fixed with respect to the laboratory frame $\mathcal{S}$, it is necessary to rotate at the same time the intermediate configuration $\mathcal{C}_{\text{inter}}$. The rotation needed is then included into elastic transformation $\mathbf{F^e}$. On the other hand, the parameters (vectors and tensors) are expressed with respect to the laboratory frame $\mathcal{S}$. To ensure the double objectivity (invariance under change of frame on the current configuration $\mathcal{C}_t$, and invariance under rotation

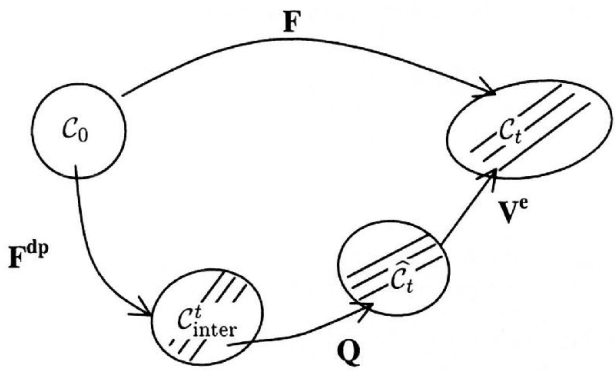

FIG. 4. Intermediate configuration as pseudo-material configuration.

of the intermediate configuration $\mathcal{C}_{\text{inter}}$) of the constitutive model, derivatives in the motion of the matter with respect to the anisotropy axes $\mathcal{A}$ are required [14]. Interference effects of the rotation of anisotropy axes $\mathcal{A}$ with respect to the laboratory frame $\mathcal{S}$ have then to be neutralized.

Let the current configuration $\mathcal{C}_t$ be virtually unstressed by a pure elastic stretching $\mathbf{V^{e-1}}$ to a new configuration called $\widehat{\mathcal{C}}_t$ (Fig. 4). $\mathbf{Q}$ denotes the orthogonal transformation from $\mathcal{C}_{\text{inter}}$ to $\widehat{\mathcal{C}}_t$ ($\mathbf{Q}$ describes the rotation of anisotropy axes $\mathcal{A}$ with respect to the laboratory fixed frame $\mathcal{S}$), and $\mathbf{W} = \dot{\mathbf{Q}}\mathbf{Q}^{\mathbf{T}}$ $\left(W_{ij} = \dot{Q}_{i\alpha}Q^T_{\alpha j}\right)$ denotes the rotation rate relative to these two configurations.
The deformation gradient $\mathbf{F}$ can be written as:

$$F_{iJ} = V^e_{ik}Q_{k\alpha}F^{dp}_{\alpha J} = V^e_{ik}\widetilde{F}^{dp}_{kJ} \tag{3.1}$$

with

$$\overset{\nabla}{\widetilde{F}}{}^{dp}_{iJ} = Q_{i\alpha}F^{dp}_{\alpha J}. \tag{3.2}$$

Introduce the derivative $\overset{\nabla}{\widetilde{\mathbf{F}}}{}^{\mathbf{dp}}$ of $\widetilde{\mathbf{F}}^{\mathbf{dp}}$, objective under any rotation of the intermediate configuration $\mathcal{C}_{\text{inter}}$ as follows:

$$\overset{\nabla}{\widetilde{F}}{}^{dp}_{iJ} = Q_{i\alpha}\dot{F}^{dp}_{\alpha J} = \dot{\widetilde{F}}^{dp}_{iJ} - W_{ik}\widetilde{F}^{dp}_{kJ} \tag{3.3}$$

and denote $\hat{\mathbf{l}}^{\mathbf{dp}}$ the objective damage-plastic velocity gradient:

$$\hat{l}^{dp}_{ij} = Q_{i\alpha}l^{dp}_{\alpha\beta}Q^{dpT}_{\beta j} = \tilde{l}^{dp}_{ij} - W_{ij} \qquad \text{with} \quad \begin{cases} l^{dp}_{\alpha\beta} = \dot{F}^{dp}_{\alpha I}F^{dp-1}_{I\beta}, \\ \tilde{l}^{dp}_{ij} = \dot{\widetilde{F}}^{dp}_{iK}\widetilde{F}^{dp-1}_{Kj}. \end{cases} \tag{3.4}$$

The velocity gradient $\mathbf{l}$ can thus be expressed by:

$$l_{ij} = \dot{F}_{iK}F^{-1}_{Kj} = \dot{V}^e_{ik}V^{e-1}_{kj} + V^e_{im}\dot{\tilde{F}}^{dp}_{mL}\tilde{F}^{dp-1}_{Lp}V^{e-1}_{pj} = \overset{\nabla}{V}{}^e_{ik}V^{e-1}_{kj} + W_{ij} + V^e_{im}\hat{l}^{dp}_{mp}V^{e-1}_{pj} \tag{3.5}$$

where

$$\overset{\nabla}{V}{}^e_{ij} = \dot{V}^e_{ij} - W_{ik}V^e_{kj} + V^e_{ip}W_{pj}. \tag{3.6}$$

As objective derivatives (3.3), (3.4) and (3.6) are constructed with the orthogonal tensor $\mathbf{W}$, they will be called rotational derivatives.

The decomposition of the velocity gradient $\mathbf{l}$ (3.5) into a symmetric part, the strain rate $\mathbf{d}$, and an antisymmetric part, the spin $\boldsymbol{\omega}$, yields:

$$\begin{aligned} d_{ij} &= \left(\overset{\nabla}{V}{}^e_{ik}V^{e-1}_{kj}\right)^S + \left(V^e_{im}\hat{l}^{dp}_{mp}V^{e-1}_{pj}\right)^S, \\ \omega_{ij} &= W_{ij} + \left(\overset{\nabla}{V}{}^e_{ik}V^{e-1}_{kj}\right)^{AS} + \left(V^e_{im}\hat{l}^{dp}_{mp}V^{e-1}_{pj}\right)^{AS}. \end{aligned} \tag{3.7}$$

The elastic strain rate $\mathbf{d^e}$ and spin $\boldsymbol{\omega}^{\mathbf{e}}$, and the inelastic strain rate $\mathbf{d^{dp}}$ and spin $\boldsymbol{\omega}^{\mathbf{dp}}$ are extracted from (3.7) as follows:

$$\begin{aligned} d^e_{ij} &= \left(\overset{\nabla}{V}{}^e_{ik}V^{e-1}_{kj}\right)^S \\ \omega^e_{ij} &= \left(\overset{\nabla}{V}{}^e_{ik}V^{e-1}_{kj}\right)^{AS} \end{aligned} \tag{3.8}$$

and

$$\begin{aligned} d^{dp}_{ij} &= \left[V^e_{im}\tilde{d}^{dp}_{mp}V^{e-1}_{pj}\right]^S + \left[V^e_{in}\hat{\omega}^{dp}_{nq}V^{e-1}_{qj}\right]^S \\ \omega^{dp}_{ij} &= \left[V^e_{im}\tilde{d}^{dp}_{mp}V^{e-1}_{pj}\right]^{AS} + \left[V^e_{in}\hat{\omega}^{dp}_{nq}V^{e-1}_{qj}\right]^{AS} \end{aligned}$$

where

$$\begin{aligned} \tilde{d}^{dp}_{ij} &= \left(\tilde{l}^{dp}_{ij}\right)^S = \left(\hat{l}^{dp}_{ij}\right)^S, \\ \hat{\omega}^{dp}_{ij} &= \left(\hat{l}^{dp}_{ij}\right)^{AS}. \end{aligned} \tag{3.9}$$

According to (3.7) and (3.8), the total strain rate $\mathbf{d}$ and spin $\boldsymbol{\omega}$ are given by:

$$\begin{aligned} d_{ij} &= d^e_{ij} + d^{dp}_{ij}, \\ \omega_{ij} &= W_{ij} + \omega^e_{ij} + \omega^{dp}_{ij}. \end{aligned} \tag{3.10}$$

The rotation rate $\mathbf{W}$ of the damage tensor eigenvectors (anisotropy axes) is obtained from $(3.10)_2$ by:

$$W_{ij} = \omega_{ij} - \left(\omega^e_{ij} + \omega^{dp}_{ij}\right). \tag{3.11}$$

As previously written by MANDEL [14], constitutive relations for anisotropic media need not only the definition of the strain rate but also that of the spin. The laws concerning $\boldsymbol{\omega}^{\mathbf{e}}$ and $\boldsymbol{\omega}^{\mathbf{dp}}$ are indeed required to achieve the calculation of the rotational derivatives (see also DAFALIAS [18]).

3.2. Constitutive model

The state of the material is described at the intermediate configuration $\mathcal{C}_{\text{inter}}$ employing the following variables:

- elastic right Cauchy-Green tensor $C^e_{\alpha\beta} = F^{eT}_{\alpha i} F^e_{i\beta} = U^e_{\alpha\gamma} U^e_{\gamma\beta}$
- absolute "regular" temperature T
- scalar isotropic strain-hardening variable p
- internal damage variable $D_{\alpha\beta} = d.n_\alpha n_\beta$ with $d = d(T^*, ...)$.

When the corresponding state variables are expressed in the current configuration $\mathcal{C}_t$, they must be invariant under rotation of the intermediate configuration $\mathcal{C}_{\text{inter}}$. The elastic left Cauchy-Green tensor $\mathbf{b}^{\mathbf{e}}$ satisfies this condition.

Anisotropy evolves during the inelastic transformation $\mathbf{F}^{\mathbf{dp}}$. Through a rotation $\mathbf{Q}$ of the intermediate configuration $\mathcal{C}_{\text{inter}}$, the vector $\mathbf{n}$ is transformed into $\widetilde{\mathbf{n}}$ as $\widetilde{\mathbf{n}} = \mathbf{Q}\mathbf{n}$ $(\widetilde{n}_i = Q_{i\alpha} n_\alpha)$. Then

$$D_{\alpha\beta} = d \cdot n_\alpha n_\beta = d Q^T_{\alpha i} \widetilde{n}_i Q^T_{\beta j} \widetilde{n}_j = d Q^T_{\alpha i} \widetilde{n}_i \widetilde{n}_j Q_{j\beta} = Q^T_{\alpha i} \widetilde{D}_{ij} Q_{j\beta}.$$

Consider the new damage variable $\widetilde{\mathbf{D}}$ invariant under rotation of the intermediate configuration $\mathcal{C}_{\text{inter}}$ as:

$$\widetilde{D}_{ij} = d\widetilde{n}_i \widetilde{n}_j = Q_{i\alpha} D_{\alpha\beta} Q^T_{\beta j}. \tag{3.12}$$

The state of the material may be described at the current configuration $\mathcal{C}_t$ employing the following variables:

- elastic left Cauchy-Green tensor $b^e_{ij} = F^e_{i\alpha} F^{eT}_{\alpha j} = V^e_{ik} V^e_{kj}$
- absolute "regular" temperature T
- scalar isotropic strain hardening variable p
- internal damage variable $\widetilde{D}_{ij} = d\widetilde{n}_i \widetilde{n}_j = Q_{i\alpha} D_{\alpha\beta} Q^T_{\beta j}$

The objective rotational derivative of $\widetilde{\mathbf{D}}$ (3.12) is obtained by neutralizing the rotation $\mathbf{Q}$:

$$\overset{\nabla}{\widetilde{D}}_{ij} = Q_{i\alpha} \dot{D}_{\alpha\beta} Q^T_{\beta j} = \dot{\widetilde{D}}_{ij} - W_{ik} \widetilde{D}_{kj} + \widetilde{D}_{ip} W_{pj}. \tag{3.13}$$

The thermo-elastic response of the anisotropic medium is supposed to be described by a thermodynamic potential, namely the free energy per unit unstressed volume $\rho^p\psi(\mathbf{C^e}, T; p, \mathbf{D})$, where ρ^p represents the density in the intermediate configuration and $\psi(\mathbf{C^e}, T; p, \mathbf{D})$ the specific free energy. Assuming incompressible inelastic deformation $\left(\det \mathbf{F^{dp}} = 1\right)$, initial and unstressed volume are equal, then $\rho_0\psi(\mathbf{C^e}, T; p, \mathbf{D}) = \rho^p\psi(\mathbf{C^e}, T; p, \mathbf{D})$, where ρ_0 represents the initial density. Material frame-indifference requirement is ensured through the invariance of the thermodynamic potential by any rotation of the intermediate configuration:

$$\rho_0\psi\left(\mathbf{C^e}, T; p, \mathbf{D}\right) = \rho_0\psi\left(\mathbf{QC^eQ^T}, T; p, \mathbf{QDQ^T}\right) = \rho_0\psi\left(\mathbf{b^e}, T; p, \widetilde{\mathbf{D}}\right).$$

The free energy per unit initial volume is further decomposed into a reversible part $\rho_0\psi^e(\mathbf{b^e}, T; \widetilde{\mathbf{D}})$, namely the elastic potential, and a stored energy part $\rho_0\psi^p(T; p, \widetilde{\mathbf{D}})$ as follows:

$$\rho_0\psi\left(\mathbf{b^e}, T; p, \widetilde{\mathbf{D}}\right) = \rho_0\psi^e\left(\mathbf{b^e}, T; \widetilde{\mathbf{D}}\right) + \rho_0\psi^p\left(T; p, \widetilde{\mathbf{D}}\right). \tag{3.14}$$

The elastic potential includes the initial isotropic linear thermo-elasticity of the sound material and damage-induced anisotropic elastic effects in the degraded material. It is constructed from the theory of isotropic scalar functions of several tensorial arguments (see BOEHLER [19]). The elastic degradation is described as dependent on $\widetilde{\mathbf{D}}$, thus comprising damage-induced orthotropy effects via two terms involving material constants a and b below, see also DRAGON *et al.* [13]. It is assumed that possible interactions between different band clusters are not taken into account. The form (3.15) below is thus limited to the first order in $\widetilde{\mathbf{D}}$.

The elastic potential is assumed in the form:

$$\rho_0\psi^e = \frac{\lambda}{2}e^e_{ii}e^e_{jj} + \mu e^e_{ij}e^e_{ji} - \alpha K e^e_{ii}\Delta T - \frac{\rho_0 C}{2T_0}\Delta T^2 - a e^e_{kk}e^e_{ij}\widetilde{D}_{ji} - 2b e^e_{ij}e^e_{jk}\widetilde{D}_{ki} \tag{3.15}$$

with

$$e^e_{ij} = g\left(b^e_{ij}\right), \qquad \Delta T = T - T_0, \qquad K = \frac{3\lambda + 2\mu}{3},$$

where $\mathbf{e^e}$ represents a spatial elastic strain measure, a function of $\mathbf{b^e}$ (see Eq. (3.23) below), which satisfies the hypotheses mentioned above concerning the elastic potential under the assumption of small elastic strains. The expression of corresponding stress tensor is given in Eq. $(3.26)_1$ below. In this context, λ and μ represent Lamé's coefficients, K the bulk modulus, α the thermal dilatation coefficient, ρ_0 the initial density, C the heat capacity, a and b the constants

mentioned above related to elastic energy degradation caused by adiabatic shear banding.

The stored energy reflects the competition that takes place inside the material between hardening and softening. Hardening is a consequence of the micromechanisms of "regular" plasticity, while softening is due to heating on the one hand and to current ASB-related damage on the other one. During their evolution (formation and propagation), ASB modify internal stresses. In this sense, one can assume that damage acts much like temperature to release the stored energy. These considerations justify the choice of a multiplicative decomposition of the hardening into respective heating and damage contributions. Note that in the expression (3.16) below, the introduction in the stored energy of the 2nd invariant of the damage variable $\widetilde{\mathbf{D}}$ allows to produce some effects of band interaction.

The stored energy is written as follows:

$$\rho_0\psi^p = R_\infty\left[p+\frac{1}{k}\exp(-kp)\right]\exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{ii}-\frac{d_2}{2}\widetilde{D}_{ij}\widetilde{D}_{ji}\right) \tag{3.16}$$

where R_∞ represents the saturation stress, k the plastic hardening parameter linked to the initial hardening modulus, γ the thermal softening parameter, d_1 and d_2 the damage (ASB)-related softening constants.

A model consistent with irreversible thermodynamic framework should satisfy the Clausius-Duhem dissipation inequality. The latter is written below in the current configuration:

$$\mathcal{D}_{\text{int}} = \sigma_{ij}d_{ji} - \rho\left(\dot{\psi}+s\dot{T}\right) \geq 0 \tag{3.17}$$

where $\boldsymbol{\sigma}$ represents the thermo-elastic (reversible) Cauchy stress tensor, ρ the current density, and s the entropy.

Chain rule applied for differentiation of the free energy gives:

$$\dot{\psi} = \frac{\partial\psi}{\partial b^e_{ij}}\dot{b}^e_{ji} + \frac{\partial\psi}{\partial T}\dot{T} + \frac{\partial\psi}{\partial p}\dot{p} + \frac{\partial\psi}{\partial\widetilde{D}_{ij}}\dot{\widetilde{D}}_{ji}\,. \tag{3.18}$$

Nevertheless, the invariance of $\dot{\psi}$ requires objective derivatives for the tensors. To avoid surplus contribution to dissipated energy, rotational derivatives are used following DOGUI and SIDOROFF [20]:

$$\dot{\psi} = \frac{\partial\psi}{\partial b^e_{ij}}\overset{\nabla}{b}{}^e_{ji} + \frac{\partial\psi}{\partial T}\dot{T} + \frac{\partial\psi}{\partial p}\dot{p} + \frac{\partial\psi}{\partial\widetilde{D}_{ij}}\overset{\nabla}{\widetilde{D}}_{ji}\,. \tag{3.19}$$

In the foregoing, the derivative $\overset{\nabla}{\mathbf{b}^e}$ is related to the strain rate $\mathbf{d}$ by:

$$\overset{\nabla}{b}{}^e_{ij} = \left(\overset{\nabla}{V}{}^e_{ik}V^e_{kj}\right) = 2V^e_{ik}d_{kl}V^e_{lj} - \left(b^e_{im}\hat{l}^{dp}_{mj} + \hat{l}^{dp}_{in}b^e_{nj}\right). \tag{3.20}$$

Gibbs relation and Clausius-Duhem inequality are finally written as:

$$
\begin{aligned}
\rho\dot{\psi} &= -\rho s\dot{T} + \sigma_{ij}\left(d_{ji} - \tilde{d}^{dp}_{ji}\right) + R\dot{p} - \widetilde{K}_{ij}\overset{\nabla}{\widetilde{D}}_{ji}\,, \\
\mathcal{D}_{\text{int}} &= \sigma_{ij}\tilde{d}^{dp}_{ji} - R\dot{p} + \widetilde{K}_{ij}\overset{\nabla}{\widetilde{D}}_{ji} \geq 0,
\end{aligned}
\tag{3.21}
$$

where $\boldsymbol{\sigma}$ represents the thermo-elastic Cauchy stress tensor, R the isotropic hardening conjugate force, $\widetilde{\mathbf{K}}$ the damage conjugate force, and s the entropy.

The conjugate forces are derived from the thermodynamic potential:

$$
\begin{aligned}
\tau_{ij} &= J\sigma_{ij} = 2\rho_0 V^e_{ik}\frac{\partial\psi}{\partial b^e_{km}}V^e_{mj} = 2\rho_0 b^e_{ip}\frac{\partial\psi}{\partial b^e_{pj}}\,, \\
r &= JR = \rho_0\frac{\partial\psi}{\partial p}\,, \\
\widetilde{k}_{ij} &= J\widetilde{K}_{ij} = -\rho_0\frac{\partial\psi}{\partial\widetilde{D}_{ij}}\,, \\
\rho_0 s &= -\rho_0\frac{\partial\psi}{\partial T}\,,
\end{aligned}
\tag{3.22}
$$

where τ represents the thermo-elastic Kirchhoff stress tensor, and J the Jacobian determinant of $\mathbf{F}$.

As stated above, the class of materials considered here implies small elastic strains. The elastic strain measure $\mathbf{e^e}$ is chosen herein as follows:

$$
e^e_{ij} = \frac{1}{2}\ln b^e_{ij} = \ln V^e_{ij}\,. \tag{3.23}
$$

Derivation of $\mathbf{e^e}$ yields an equality between the rotational derivative $\overset{\nabla}{\mathbf{e}}^{\mathbf{e}}$ and the elastic strain rate $\mathbf{d^e}$:

$$
\overset{\nabla}{e}{}^e_{ij} = d^e_{ij} = \dot{e}^e_{ij} - W_{ik}e^e_{kj} + e^e_{ip}W_{pj}\,. \tag{3.24}
$$

On the other hand, the thermo-elastic Kirchhoff stress tensor is simply expressed as follows:

$$
\tau_{ij} = \rho_0\frac{\partial\psi}{\partial e^e_{ij}}\,. \tag{3.25}
$$

The conjugate forces (3.22) are henceforth expressed by:

$$
\begin{aligned}
\tau_{ij} &= \lambda e^e_{kk}\delta_{ij} + 2\mu e^e_{ij} - \alpha K \Delta T \delta_{ij} \\
&\quad - a\left(e^e_{mn}\widetilde{D}_{nm}\delta_{ij} + e^e_{kk}\widetilde{D}_{ij}\right) - 2b\left(e^e_{ik}\widetilde{D}_{kj} + \widetilde{D}_{ik}e^e_{kj}\right), \\
r &= R_\infty\left[1 - \exp\left(-kp\right)\right]\exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right), \\
\tilde{k}_{ij} &= a e^e_{kk}e^e_{ij} + 2b e^e_{ik}e^e_{kj} + R_\infty\left[p + \frac{1}{k}\exp(-kp)\right] \\
&\quad \cdot \exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right)\left[d_1\delta_{ij} + d_2\widetilde{D}_{ij}\right], \\
\rho_0 s &= \alpha K e^e_{kk} + \frac{\rho C}{T_0}\Delta T \\
&\quad + \gamma R_\infty\left[p + \frac{1}{k}\exp(-kp)\right]\exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right).
\end{aligned}
\tag{3.26}
$$

Isotropic heating and anisotropic damage contribute to reduction of the stress level $\tau_{ij}\left(\mathbf{e}^{\mathbf{e}}, T; \widetilde{\mathbf{D}}\right)$ $(3.26)_1$. Positive constants a and b contribute both to reduction of the Young's modulus, while b is alone related to the decrease of the shear modulus (see also Sec. 5).

Without heating and damage (isothermal conditions in quasi-static configuration), the conjugate force $r(T; p, \widetilde{\mathbf{D}})$ in $(3.26)_2$, relative to isotropic hardening, tends to the saturation stress $R_\infty \exp(-\gamma T_0)$. This force increases during pure hardening but decreases with heating and damage, describing the competition between hardening and softening.

The damage conjugate force $\widetilde{\mathbf{k}}(\mathbf{e}^{\mathbf{e}}, T; p, \widetilde{\mathbf{D}})$ — the energy release rate with respect to $\widetilde{\mathbf{D}}$ — $(3.26)_3$ includes the first contribution from the reversible part of the free energy, and the second one from the stored energy. The corresponding terms represent respectively elastic and stored energy release rates. It is noteworthy that both contributions to the damage conjugate force exist before damage inception. It is assumed that a finite supply of energy is necessary to activate the damage process.

The objective formulation of the incremental constitutive model can be written in a compact form as follows:

$$
\begin{Bmatrix} +\overset{\nabla}{\tau}_{ij} \\ +\dot{r} \\ -\overset{\nabla}{\tilde{k}}_{ij} \\ -\rho_0\dot{s} \end{Bmatrix} = \begin{bmatrix} C_{ijkl} & 0 & E_{ijkl} & J_{ij} \\ 0 & Q & A_{kl} & S \\ E_{ijkl} & A_{ij} & L_{ijkl} & V_{ij} \\ J_{kl} & S & V_{kl} & X \end{bmatrix} \begin{Bmatrix} d_{kl} - \widetilde{d}^{dp}_{kl} \\ \dot{p} \\ \overset{\nabla}{\widetilde{D}}_{kl} \\ \dot{T} \end{Bmatrix}. \tag{3.27}
$$

with

$$C_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial e^e_{kl}}; \qquad E_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial \widetilde{D}_{kl}}; \qquad J_{ij} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial T}; \qquad Q = \rho_0 \frac{\partial^2 \psi}{\partial p^2}$$

and

$$S = \rho_0 \frac{\partial^2 \psi}{\partial p \partial T}; \qquad A_{ij} = \rho_0 \frac{\partial^2 \psi}{\partial p \partial \widetilde{D}_{ij}}; \qquad L_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial \widetilde{D}_{ij} \partial \widetilde{D}_{kl}};$$

$$V_{ij} = \rho_0 \frac{\partial^2 \psi}{\partial \widetilde{D}_{ij} \partial T}; \qquad X = \rho_0 \frac{\partial^2 \psi}{\partial T^2}$$

(see Appendix A for further details).

Since we have assumed small elastic strains ($V^e_{ij} \approx \delta_{ij} + \varepsilon_{ij}$ with $\varepsilon_{ij}\varepsilon_{ji} \ll 1$), expressions (3.8) are reduced to:

$$\text{(3.28)} \qquad \begin{cases} d^e_{ij} = \overset{\nabla}{V}{}^e_{ij} \\ \omega^e_{ij} = 0 \end{cases} \qquad \begin{cases} d^{dp}_{ij} = \widetilde{d}^{dp}_{ij}, \\ \omega^{dp}_{ij} = \widehat{\omega}^{dp}_{ij}. \end{cases}$$

As a consequence, the rotation rate (3.11), needed for the rotational derivatives, becomes:

$$\text{(3.29)} \qquad W_{ij} = \omega_{ij} - \omega^{dp}_{ij}.$$

As stated before, the constitutive model requires a law specifying $\omega^{\mathbf{dp}}$ in addition to the conventional complementary laws.

Another consequence of the small elastic strains assumption concerns the form (3.27) which becomes:

$$\text{(3.30)} \qquad \begin{Bmatrix} +\overset{\nabla}{\tau}_{ij} \\ +\dot{r} \\ -\overset{\nabla}{\tilde{k}}_{ij} \\ -\rho_0 \dot{s} \end{Bmatrix} = \begin{bmatrix} C_{ijkl} & 0 & E_{ijkl} & J_{ij} \\ 0 & Q & A_{kl} & S \\ E_{ijkl} & A_{ij} & L_{ijkl} & V_{ij} \\ J_{kl} & S & V_{kl} & X \end{bmatrix} \begin{Bmatrix} d^e_{kl} \\ \dot{p} \\ \overset{\nabla}{\widetilde{D}}_{kl} \\ \dot{T} \end{Bmatrix}.$$

The dissipation can be decomposed into a "regular" part directly linked to plasticity and a "singular" part resulting from band formation:

$$\text{(3.31)} \qquad \mathcal{D}_{\text{int}} = \mathcal{D}_{\text{reg}} + \mathrm{D}_{\text{sing}}.$$

The respective contributions are as follows:

$$\text{(3.32)} \qquad \begin{aligned} \mathcal{D}_{\text{reg}} &= \sigma_{ij} d^p_{ji} - R\dot{p}, \\ \mathcal{D}_{\text{sing}} &= \sigma_{ij} d^d_{ji} + F_{ij} \overset{\nabla}{\widetilde{D}}_{ji}, \end{aligned}$$

where $\mathbf{d}^{\mathbf{p}}$ represents the "regular" plastic strain rate, and $\mathbf{d}^{\mathbf{d}}$ the "singular" damage-induced strain rate.

The effects of "singular" heating localized inside the band cluster are included, by definition of the damage variable (2.1)–(2.2), in the scalar damage density d^{α} (2.2), evolving with the ongoing deterioration. "Regular" heating caused by plasticity outside the bands is then expressed by the common relation established with the adiabaticity assumption:

$$\rho_0 C\dot{T} = \sigma_{ij} d^p_{ji} - R\dot{p}. \tag{3.33}$$

One may distinguish three stages during the deformation progress: before the onset of localization, "regular" plasticity is the only dissipative mechanism; just after the onset of localization, both mechanisms, namely "regular" plasticity and "singular" damage coexist; when localization advances, ASB damage process becomes progressively the prevalent dissipative mechanism. Using a single yield function that includes both the plasticity and damage effects, seems to be suitable to favour such a chronology in the evolution of "regular" and "singular" variables.

The following extended form of the plasticity and damage loading function $\mathcal{F}$ is postulated:

$$\mathcal{F}\left(\tau_{ij}, r, \tilde{k}_{ij}\right) = \hat{J}_2^s\left(\tau_{ij}, \tilde{k}_{ij}\right) - (R_0 + r), \tag{3.34}$$

where the generalized 2nd invariant $\hat{J}_2^s\left(\tau, \widetilde{\mathbf{k}}\right)$ incorporates the damage conjugate force $\widetilde{\mathbf{k}}\left(\widetilde{\mathbf{D}}, ...\right)$ as follows:

$$\hat{J}_2^s\left(\tau_{ij}, \tilde{k}_{ij}\right) = \sqrt{\frac{3}{2} s_{ij} P_{ijkl}\left(\tilde{k}_{mn}\right) s_{kl}}. \tag{3.35}$$

In (3.35) $\mathbf{s}$ represents the deviatoric part of the Kirchhoff stress tensor, and $\mathbf{P}\left(\widetilde{\mathbf{k}}\right)$ the 4th order tensor inducing anisotropy of plastic flow.

The tensor $\mathbf{P}\left(\widetilde{\mathbf{k}}\right)$, see (3.37) below, includes the first term relative to conventional plasticity without damage and the second one relative to damage-induced effects on the plastic flow. The evolution laws (3.43), which are derived from the normality rule, require by definition the collinearity of the "regular" plastic strain rate $\mathbf{d}^{\mathbf{p}}$ to the deviatoric part $\mathbf{s}$ of the Kirchhoff stress tensor, the collinearity of the "singular" damage-induced strain rate $\mathbf{d}^{\mathbf{d}}$ to the orientation tensor $\mathbf{M}$ (according to $(2.3)_1$), and finally the collinearity of the damage rate $\overset{\nabla}{\widetilde{\mathbf{D}}}$ to the orientation tensor $\mathbf{N}$ for conservative damage growth configuration

considered here (according to $(2.1)_1$). Conjugate forces $\left(\mathbf{s}, \widetilde{\mathbf{k}}\right)$ and "orientation" tensors $(\mathbf{s}, \mathbf{M}, \mathbf{N})$ are then associated in the generalized 2^{nd} invariant (3.35) to satisfy such conditions. The continuity of stress at the onset of damage is preserved. In the expression of $\mathbf{P}$, the damage driving force $\widetilde{\mathbf{k}}$ intervenes via the expression $\text{Tr}\left(\widetilde{\mathbf{k}}^{+}\mathbf{N}\right)$, where $\text{Tr}\left(\widetilde{\mathbf{k}}^{+}\mathbf{N}\right)$ represents the difference between the current value $\text{Tr}\left(\widetilde{\mathbf{k}}\mathbf{N}\right)$ and the corresponding one at the incipience of damage $k_{\text{inc}} = \text{Tr}\left(\widetilde{\mathbf{k}}\mathbf{N}\right)_{inc}$:

$$\tilde{k}^{+}_{ij} N_{ji} = \left\langle \tilde{k}_{ij} N_{ji} - k_{\text{inc}} \right\rangle, \tag{3.36}$$

where the bracket $\langle \cdot \rangle$ defines the ramp function. To determine k_{inc}, an auxiliary analysis based on perturbation method will be conducted in Section 4 for a particular loading path.

On the other hand, to ensure the concomitance of both damage-induced rates $\mathbf{d}^{\mathbf{d}}$ and $\overset{\nabla}{\widetilde{\mathbf{D}}}$, the polynomial in $\text{Tr}\left(\widetilde{\mathbf{k}}^{+}\mathbf{N}\right)$ specified below in (3.37) starts with the exponent $q = 2$ (see $(3.43)_2$ and $(3.43)_4$ below).

The 4^{th} order tensor $\mathbf{P}\left(\widetilde{\mathbf{k}}\right)$ is finally represented as follows:

$$P_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + 2\sum_{q=2}^{N} \eta_q \left(\tilde{k}^{+}_{mn} N_{nm}\right)^q M_{ij} M_{kl}\,. \tag{3.37}$$

The function R_0 in (3.34), which represents the radius of the Huber-Von Mises cylinder without hardening in the stress space, must account for heating and damage softening. A form close to the hardening conjugate force $(3.26)_2$ is adopted:

$$R_0 = R_i \exp(-\gamma T) \exp\left(-d_1 \widetilde{D}_{kk} - \frac{d_2}{2} \widetilde{D}_{mn} \widetilde{D}_{nm}\right), \tag{3.38}$$

where R_i represents the internal stress, γ the thermal softening parameter, d_1 and d_2 the damage (ASB) softening parameters. The inelasticity criterion $\mathcal{F} = 0$ is assumed. The viscoplastic flow and (viscous) damage growth domain is thus $\mathcal{F} \geq 0$.

The existence of a viscoplastic potential of PERZYNA's type [21] is assumed:

$$\phi_p^c = \frac{Y}{n+1} \left\langle \frac{\mathcal{F}}{Y} \right\rangle^{n+1} \tag{3.39}$$

where $\mathcal{F}$ represents the yield function, Y and n viscous parameters relative to "regular" plasticity, and the bracket $\langle \cdot \rangle$ the ramp function. Time-dependent

shear banding (damage mechanism considered here) is an evident consequence of thermo-viscoplastic flow. The viscous damage potential is thus chosen close to the plastic one (3.39):

$$\phi_d^c = \frac{Z}{m+1}\left\langle \frac{\mathcal{F}}{Z} \right\rangle^{m+1} \tag{3.40}$$

where $\mathcal{F}$ represents the yield function, Z and m viscous parameters relative to "singular" damage, and the bracket $\langle\cdot\rangle$ is the ramp function.

Evolution laws are consequently derived from the normality rule:

$$\begin{aligned} d_{ij}^{dp} &= d_{ij}^{p} + d_{ij}^{d} = \frac{\partial \phi_p^c}{\partial \tau_{ij}} = \Lambda^p \frac{\partial \mathcal{F}}{\partial \tau_{ij}}\,; \\ -\dot{p} &= \frac{\partial \phi_p^c}{\partial r} = \Lambda^p \frac{\partial \mathcal{F}}{\partial r}\,; \qquad \overset{\nabla}{\tilde{D}}_{ij} = \frac{\partial \phi_d^c}{\partial \tilde{k}_{ij}} = \Lambda^d \frac{\partial \mathcal{F}}{\partial \tilde{k}_{ij}} \end{aligned} \tag{3.41}$$

with the viscoplasticity and viscous damage respective multipliers expressed by:

$$\Lambda^p = \left\langle \frac{\partial \phi_p^c}{\partial \mathcal{F}} \right\rangle = \left\langle \frac{\mathcal{F}}{Y} \right\rangle^n ; \qquad \Lambda^d = \left\langle \frac{\partial \phi_d^c}{\partial \mathcal{F}} \right\rangle = \left\langle \frac{\mathcal{F}}{Z} \right\rangle^m . \tag{3.42}$$

The corresponding fluxes are finally written as follows:

$$\begin{aligned} d_{ij}^{p} &= \frac{3}{2}\Lambda^p \frac{s_{ij}}{\widehat{J}_2^s}\,, \\ d_{ij}^{d} &= 3\Lambda^p \frac{\sum_{q=2}^{N} \eta_q \left(\tilde{k}_{mn}^{+} N_{nm}\right)^q s_{kl} M_{kl}}{\widehat{J}_2^s} M_{ij}\,, \\ \dot{p} &= \Lambda^p, \\ \overset{\nabla}{\tilde{D}}_{ij} &= \frac{3}{2}\Lambda^d \frac{\sum_{q=2}^{N} q \cdot \eta_q \left(\tilde{k}_{mn}^{+} N_{nm}\right)^{q-1} (s_{kl} M_{kl})^2}{\widehat{J}_2^s} N_{ij}\,. \end{aligned} \tag{3.43}$$

As discussed above, the rates $\mathbf{d^p}$, $\mathbf{d^d}$ and $\overset{\nabla}{\tilde{\mathbf{D}}}$ are respectively collinear to $\mathbf{s}$, $\mathbf{M}$ and $\mathbf{N}$. The adiabatic shear banding process which generates the damage-induced strain rate $\mathbf{d^d}$ modifies the initial direction of the inelastic strain rate $\mathbf{d^{dp}}$. The norms of the damage-induced rates $\mathbf{d^d}$ and $\overset{\nabla}{\tilde{\mathbf{D}}}$ contain both a part relative to the damage conjugate force $\tilde{\mathbf{k}}$ (via the expression $\mathrm{Tr}\left(\tilde{\mathbf{k}}^{+}\mathbf{N}\right)$) and another part relative to the resolved shear stress $\tau_{\mathrm{res}} = \mathrm{Tr}\,(\mathbf{sM})$ (in the band cluster plane).

The damage conjugate force $\tilde{\mathbf{k}}$ is actually the preponderant driving force of the damage-induced strain rate $\mathbf{d}^{\mathbf{d}}$ (see the expression $(3.43)_2$ above), while the damage conjugate force $\tilde{\mathbf{k}}$ and the resolved shear stress τ_{res} keep approximately the same weight in the expression $(3.43)_4$ governing the magnitude of the damage rate $\overset{\nabla}{\tilde{\mathbf{D}}}$, recalling that damage is primarily the consequence of a shearing process.

Let the inelastic velocity gradient $\mathbf{l}^{\mathbf{dp}}$ be decomposed into a "regular" contribution $\mathbf{l}^{\mathbf{p}}$ and a "singular" one $\mathbf{l}^{\mathbf{d}}$:

$$l_{ij}^{dp} = l_{ij}^{p} + l_{ij}^{d}\,. \tag{3.44}$$

In the absence of damage ($\mathbf{l}^{\mathbf{d}} = \mathbf{0}$), the "regular" structure of matter can be supposed to be approximately statistically isotropic, what implies that $\omega^{\mathbf{p}} = \mathbf{0}$, see MANDEL [22]. The rate $\mathbf{W}$ is in this case equal to the spin ω: rotational derivatives are then simply the Zaremba-Jaumann derivatives. In the presence of damage, the damage-induced velocity gradient $\mathbf{l}^{\mathbf{d}}$ generates the spin $\omega^{\mathbf{d}}$. Assuming that the effects of the distorsion caused by the presence of ASB are concentrated in their close vicinity, "regular" matter is supposed to be globally weakly affected. In this sense, the "regular" plastic spin $\omega^{\mathbf{p}}$ can be neglected with respect to the "singular" damage-induced spin $\omega^{\mathbf{d}}$. The rotation rate (3.29) is thus reduced to:

$$W_{ij} = \omega_{ij} - \omega_{ij}^{d}. \tag{3.45}$$

The analogy drawn in Section 2 between a band cluster and a "super-dislocation" is used here again to postulate the "singular" contribution $\mathbf{l}^{\mathbf{d}}$ as:

$$l_{ij}^{d} \propto \sum_{\alpha} \dot{\gamma}^{\alpha} g_i^{\alpha} n_j^{\alpha}. \tag{3.46}$$

The partition of the damage-induced velocity gradient $\mathbf{l}^{\mathbf{d}}$ (3.46) gives the damage-induced strain rate $\mathbf{d}^{\mathbf{d}}$ and the damage-induced spin $\omega^{\mathbf{d}}$ as follows:

$$\begin{aligned} d_{ij}^{d} &\propto \sum_{\alpha} \dot{\gamma}^{\alpha} \left(g_i^{\alpha} n_j^{\alpha}\right)^{S}, \\ \omega_{ij}^{d} &\propto \sum_{\alpha} \dot{\gamma}^{\alpha} \left(g_i^{\alpha} n_j^{\alpha}\right)^{AS}. \end{aligned} \tag{3.47}$$

According to relation $(3.43)_2$, which expresses the damage-induced strain rate $\mathbf{d}^{\mathbf{d}}$, one can express the damage-induced spin $\omega^{\mathbf{d}}$ $(3.47)_2$ as:

$$\omega_{ij}^{d} = 3\Lambda^{p} \frac{\sum_{r=2}^{N} \eta_r \left(\tilde{k}_{pq}^{+} N_{qp}\right)^{r} s_{kl} M_{kl}}{\hat{J}_2^{s}} T_{ij} \tag{3.48}$$

where

$$T_{ij} = (g_i n_j)^{AS} = \frac{1}{2}(g_i n_j - g_j n_i).$$

As stressed before, material behaviour, described via the incremental law (3.30), requires objective rotational derivatives. From the analogy of damage-induced viscoplastic deformation with finite plastic distorsion in crystals, the above evaluation of the damage-induced spin has been obtained, thus completing the constitutive relations.

4. Damage incipience via simplified perturbation analysis

The constitutive model is now completed by a damage incipience criterion based on a simplified analysis of material instability using the linear perturbation method.

The method is in general applied in the case of simple shear under constant velocity boundary conditions. Assuming negligible elastic effects, laminar viscoplastic flow and adiabatic conditions, the problem can be reduced to a one-dimensional formulation, see e.g. BAI [3], CLIFTON *et al.* [23], MOLINARI [24], and SHAWKI and CLIFTON [25]. Admitting analytical solutions, the linear perturbation method provides in this case a criterion of instability onset, which is interpreted as the incipience of the adiabatic shear banding process. Nevertheless, instability does not rigorously imply localization [24]. This means that the use of the method gives a "lower" bound of the deformation localization incipience.

An auxiliary simplified analysis performed here is intended to help to establish damage incipience threshold and its form based on more pertinent indications than the purely phenomenological formulation. The output of the analysis presented below will be limited to a particular loading path. Instead of rigorous instability search ("lower" bound for localization mentioned above), the aim is to search a more realistic ("upper" bound) evaluation for localization incipience. The hypotheses taken further favour delaying the strong localization onset with respect to the supposed instability onset.

As mentioned in Sec. 3, this auxiliary analysis allows actually to determine $k_{\text{inc}} = \text{Tr}\left(\widetilde{\mathbf{kN}}\right)_{\text{inc}}$ in (3.36), which activates the damage-related rates $\mathbf{d}^{\mathbf{d}}$ and $\overset{\nabla}{\widetilde{\mathbf{D}}}$ (see expressions $(3.43)_2$ and $(3.43)_4$), from mechanical considerations. In the absence of damage, assuming negligible elastic effects, the governing equations may be written as:

$$\tau_{ij,j} - \rho_0 \dot{v}_i = 0,$$

$$\rho_0 C \dot{T} - \kappa T_{,kk} - (J_2 - r)\dot{p} = 0, \tag{4.1}$$

$$
\begin{aligned}
\frac{1}{2}(v_{i,j}+v_{j,i})-\frac{3}{2}\dot{p}\frac{s_{ij}}{J_2} &= 0,\\
\dot{p}-\Lambda^p(\tau_{ij},p,T) &= 0,
\end{aligned}
\tag{4.1 [cont.]}
$$

where $J_2=\sqrt{\frac{3}{2}s_{ij}s_{ji}}$ and where κ represents the thermal conductivity.

Let a small perturbation $\delta U=(\delta v_i,\delta\tau_{ij},\delta p,\delta T)$ be superposed on the set of homogeneous solutions $U=(v_i,\tau_{ij},p,T)$ of the system (4.1):

$$U\Rightarrow U+\delta U \qquad \text{with} \quad \delta U\ll U.$$

Homogeneous solutions evolution is supposed to be slower than perturbations (see also KERYVIN *et al.* [26]): the system is considered to be temporarily frozen. The perturbed system can thus be studied independently.

After linearization, it takes the form:

$$
\begin{aligned}
\delta\tau_{ij,j}-\rho_0\delta\dot{v}_i &= 0,\\
\rho_0C\delta\dot{T}-\kappa\delta T_{,kk}-(\delta J_2-\delta r)\dot{p}-(J_2-r)\delta\dot{p} &= 0,\\
\frac{1}{2}(\delta v_{i,j}+\delta v_{j,i})-\frac{3}{2}\delta\dot{p}\frac{s_{ij}}{J_2}-\frac{3}{2}\dot{p}\delta\left(\frac{s_{ij}}{J_2}\right) &= 0,\\
\delta\dot{p}-\delta\Lambda^p(\tau_{ij},p,T) &= 0.
\end{aligned}
\tag{4.2}
$$

Let the perturbation have a wave-like form:

$$\delta U=\overline{U}\exp\left(\varpi t+ik\underline{n}\,\underline{x}\right)=\overline{U}\exp[\varpi_R t]\exp\left[ik\left(ct+\underline{n}\,\underline{x}\right)\right] \tag{4.3}$$

where $\overline{U}$ represents the perturbation magnitude, ϖ the wave pulsation, k the wave number, $\underline{n}$ the wave vector, ϖ_R and ϖ_I respectively the real and imaginary parts of the wave pulsation ϖ, and $c=\varpi_I/k$ the wave velocity.

According to the right-hand term of (4.3), the case $\varpi_R=0$ points the transition between the stable and unstable states:

- if $\varpi_R>0$, the perturbation increases with time;
- if $\varpi_R<0$, the perturbation decreases with time.

The objective consists in looking for the conditions of the transition from the stable state to the unstable state by studying the sign of ϖ_R.

After injecting the perturbation (4.3) into the system (4.2), one obtains:

$$
\begin{aligned}
ikn_j\overline{\tau}_{ji}-\rho_0\varpi\overline{v}_i &= 0,\\
\left(\rho_0C\varpi+\kappa k^2+S^0\dot{p}\right)\overline{T}-\dot{p}\frac{3}{2}\frac{s_{ij}\overline{\tau}_{ji}}{J_2}+\left[Q^0\dot{p}-(J_2-r)\varpi\right]\overline{p} &= 0,\\
\frac{ik}{2}\left(n_j\overline{v}_i+n_i\overline{v}_j\right)-\frac{3}{2}\frac{s_{ij}}{J_2}\varpi\overline{p}-\dot{p}G_{ijkl}\overline{\tau}_{kl} &= 0,\\
(\varpi-B)\overline{p}-P_{ij}\overline{\tau}_{ji}-E\overline{T} &= 0,
\end{aligned}
\tag{4.4}
$$

with

$$Q^0 = \frac{\partial r}{\partial p}; \qquad S^0 = \frac{\partial r}{\partial T}; \qquad G_{ijkl} = \frac{3}{2}\frac{\partial\left(\frac{s_{ij}}{J_2}\right)}{\partial \tau_{kl}};$$
$$P_{ij} = \frac{\partial \Lambda^p}{\partial \tau_{ij}}; \qquad B = \frac{\partial \Lambda^p}{\partial p}; \qquad E = \frac{\partial \Lambda^p}{\partial T}$$

(see Appendix B for further details).

The system (4.4) can be written as:

$$[\mathcal{M}]\{\overline{U}\} = \{0\}. \tag{4.5}$$

The next step consists in finding the roots ϖ from the determinant of the matrix $[\mathcal{M}]$. In the case of a thermo-viscoplastic behaviour, the determinant is a 4^{th} degree polynomial in ϖ. Solutions are not trivial and require the knowledge of the perturbation direction.

In the particular case of simple shear, where $v_1 \neq 0$ and $\tau_{12} \neq 0$, the perturbed system (4.4) takes the form:

$$\begin{aligned} ikn_2\overline{\tau}_{12} - \rho_0\varpi\overline{v}_1 &= 0, \\ \left(\rho_0 C\varpi + \kappa k^2 + S^0\dot{p}\right)\overline{T} - \sqrt{3}\dot{p}\overline{\tau}_{12} + \left[Q^0\dot{p} - \left(\sqrt{3}\tau_{12} - r\right)\varpi\right]\overline{p} &= 0, \\ ikn_2\overline{v}_1 - \sqrt{3}\varpi\overline{p} &= 0, \\ (\varpi - B)\overline{p} - \sqrt{3}\alpha\overline{\tau}_{12} - E\overline{T} &= 0, \end{aligned} \tag{4.6}$$

or otherwise

$$\begin{bmatrix} -\rho_0\varpi & ikn_2 & 0 & 0 \\ 0 & -\sqrt{3}\dot{p} & \left[Q^0\dot{p} - \left(\sqrt{3}\tau_{12} - r\right)\varpi\right] & \left(\rho_0 C\varpi + \kappa k^2 + S^0\dot{p}\right) \\ ikn_2 & 0 & -\sqrt{3}\varpi & 0 \\ 0 & -\sqrt{3}\alpha & (\varpi - B) & -E \end{bmatrix} \tag{4.7}$$
$$\times \begin{Bmatrix} \overline{v}_1 \\ \overline{\tau}_{12} \\ \overline{p} \\ \overline{T} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix}.$$

The system (4.7) can be written as:

$$[\mathcal{M}]\{\overline{U}\} = \{0\}. \tag{4.8}$$

The direction of the pertubation is obviously collinear with x_2 and the determinant of the matrix $[\mathcal{M}]$ is a 3^{rd} degree polynomial in ϖ:

$$\det[\mathcal{M}] = a_3\varpi^3 + a_2\varpi^2 + a_1\varpi^1 + a_0 \tag{4.9}$$

where

$$
\begin{aligned}
a_3 &= 3\rho_0^2 C\alpha, \\
a_2 &= \rho_0 \left[3\left(E + S^0\alpha\right)\dot{p} + k^2\left(3\kappa\alpha + C\right)\right], \\
a_1 &= k^2\left[\kappa k^2 + S^0\dot{p} - \rho_0 CB - E\left(\sqrt{3}\tau_{12} - r\right)\right], \\
a_0 &= k^2\left[\left(EQ^0 - BS^0\right)\dot{p} - \kappa k^2 B\right].
\end{aligned} \tag{4.10}
$$

Assuming adiabatic conditions ($\kappa = 0$), the coefficients (4.10) are reduced to:

$$
\begin{aligned}
a_3 &= 3\rho_0^2 C\alpha, \\
a_2 &= \rho_0 \left[3\left(E + S^0\alpha\right)\dot{p} + k^2 C\right], \\
a_1 &= k^2\left[S^0\dot{p} - \rho_0 CB - E\left(\sqrt{3}\tau_{12} - r\right)\right], \\
a_0 &= k^2\left(EQ^0 - BS^0\right)\dot{p},
\end{aligned} \tag{4.11}
$$

$$
\begin{aligned}
E + S^0\alpha &= -\alpha\frac{\partial R_0}{\partial T}, \\
EQ^0 - BS^0 &= -\alpha\frac{\partial R_0}{\partial T}Q^0,
\end{aligned} \tag{4.12}
$$

(see Appendix B for further details).

As stated previously, the idea is to delay the instability onset to approach the strong localization incipience. Adiabatic shear banding occurs as thermal softening overcomes the plastic hardening. In the constitutive model developed in Section 3, thermal softening is described through the partial derivatives of the hardening conjugate force $r\left(T; p, \widetilde{\mathbf{D}}\right)$ and of the internal stress $R_0\left(T; \widetilde{\mathbf{D}}\right)$ with respect to temperature. By neglecting the last contribution ($\partial R_0/\partial T = 0$) to thermal softening, the aforementioned delayed estimation (an "upper" bound for the instability onset) is reached without losing the mechanical consistency.

It is noteworthy that this simplification facilitates obtaining the analytical results. The expressions (4.12) become indeed zero, as also the coefficient a_0 in (4.11). The degree of the polynomial (4.9) is then equal to 2, and analytical solutions are obvious.

With the simplification $\partial R_0/\partial T = 0$ in the stability analysis, the coefficients (4.11) become:

$$
\begin{aligned}
a_3 &= 3\rho_0^2 C\alpha, \\
a_2 &= \rho_0 k^2 C, \\
a_1 &= k^2\left[S^0\dot{p} - \rho_0 CB - E\left(\sqrt{3}\tau_{12} - r\right)\right], \\
a_0 &= 0.
\end{aligned} \tag{4.13}
$$

As shown above, the determinant of the matrix $[\mathcal{M}]$ is a 2^{nd} degree polynomial in ϖ:

$$\det[\mathcal{M}] = a_3\varpi^2 + a_2\varpi + a_1 = 0. \tag{4.14}$$

The condition of instability may thus be written as:

$$\varpi > 0 \qquad \text{if and only if} \quad a_1 a_3 < 0.$$

The perturbation grows if and only if

$$3\rho_0^2 C\alpha k^2 \left[S^0\dot{p} - \rho_0 CB - E\left(\sqrt{3}\tau_{12} - r\right)\right] < 0, \tag{4.15}$$

or else, with the relations in Appendix B,

$$\frac{\partial r}{\partial p} < \frac{\left(\sqrt{3}\tau_{12} - r\right) + \dfrac{\dot{p}}{\alpha}}{\rho_0 C}\left(-\frac{\partial r}{\partial T}\right). \tag{4.16}$$

With $\dfrac{\dot{p}}{\alpha} = \dfrac{Y\dot{p}^{1/n}}{n}$, inequality (4.16) becomes:

$$\frac{\partial r}{\partial p} < \frac{\left(\sqrt{3}\tau_{12} - r\right) + \dfrac{Y\dot{p}^{1/n}}{n}}{\rho_0 C}\left(-\frac{\partial r}{\partial T}\right). \tag{4.17}$$

This condition of instability involves plastic hardening and thermal softening through the partial derivatives of the isotropic hardening conjugate force $r\,(T; p, \mathbf{D})$.

Consider another expression of inequality (4.16) as follows:

$$\mathcal{G}\left(\tau_{ij}, r, \dot{p}; \frac{\partial r}{\partial p}, \frac{\partial r}{\partial T}\right) = \sqrt{3 s_{ij} M_{ji} s_{kl} M_{lk}} - \left(r - \frac{Y\dot{p}^{1/n}}{n} + \rho_0 C \frac{\dfrac{\partial r}{\partial p}}{\left(-\dfrac{\partial r}{\partial T}\right)}\right) > 0. \tag{4.18}$$

Inequality (4.18) relates the resolved shear stress $\tau_{\text{res}} = s_{ij}M_{ji}$ to the isotropic conjugate force r, the strain rate-induced overstress $Y\dot{p}^{1/n}$, and the ratio of the plastic hardening $\partial r/\partial p$ to the thermal softening $\partial r/\partial T$.

In the present simplified analysis, the damage process is actually assumed to run as soon as $\mathcal{G}\left(\tau_{ij}, r, \dot{p}; \dfrac{\partial r}{\partial p}, \dfrac{\partial r}{\partial T}\right) = 0$. This latter condition must be interpreted as the auxiliary indicator for the damage process incipience leading to the

determination of the damage conjugate force threshold $k_{\text{inc}} = \text{Tr}\left(\widetilde{\mathbf{kN}}\right)_{\text{inc}}$ in the model of Section 3, see Eq. (3.36). Though a delay has been introduced in the instability onset, this condition is surely necessary but not sufficient, as shown in [24]. Further advanced studies involving the onset of strain localization in the presence of multiple mechanisms of inelastic deformation can be envisioned following the lines of the recent study by PETRYK [27]. The latter would necessitate adaptation to the rate-dependent constitutive framework.

It is noteworthy that the criterion (4.18) is obtained from an analysis based on the linear perturbation method, and not from an arbitrary, or purely phenomenological, damage incipience criterion.

5. Preliminary evaluation and comments on model capacities

The three-dimensional constitutive model developed in Sec. 3 is tested on a volume element (material point) loaded in simple shear in the context of adiabatic dynamic process. The time integration procedure is purely explicit and the time increment is imposed at the beginning of the analysis. The simple shear loading is applied via the velocity gradient l_{12} (Fig. 6). The damage process (strong deformation localization) is supposed to occur inside the material through the development of a single shear band pattern of normal vector $\underline{n}$ collinear with the $\underline{x}_2$ axis (Fig. 5). The calculation of k_{inc} is determined via the auxiliary method detailed in Sec. 4.

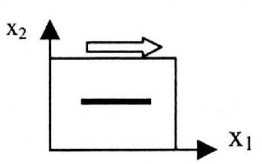

FIG. 5. Volume element containing a band.

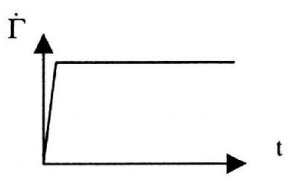

FIG. 6. Nominal shear strain rate history.

The nominal deformation gradient $\mathbf{F}$, the nominal velocity gradient $\mathbf{l}$, and the damage variable $\widetilde{\mathbf{D}}$ are given by:

$$[F] = \begin{bmatrix} 1 & \Gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad [l] = \dot{\Gamma} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [D] = d \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where $\dot{\Gamma}$ represents the nominal shear strain rate, and Γ the nominal shear strain.

In order to illustrate the model capabilities, experimental data by MARCHAND and DUFFY [5] have been chosen as general reference. The curve (Fig. 7)

they obtained from a high strain rate torsional test on a HY 100 steel tubular sample is usually used to illustrate adiabatic shear banding effects. This curve displays three consecutive stages: in the 1st stage, thermo-elastic/viscoplastic behaviour is stable; in the 2nd stage, a weak instability in flow appears; in the 3rd stage, the instability becomes strong and the deformation localizes through adiabatic shear bands. Model constants (Table 1) have been identified from these experimental data (Fig. 7). Consequently, the curve in Fig. 8 should not be considered as the one validating the model; it reproduces simply the experimental curve of Fig. 7. The discussion of model capabilities will be given below on the basis of specific additional correlations concerning the actual model, namely its response in terms of the state variables and their conjugate forces. Finally, by modifying the loading conditions given by [5], the beginning of validation will be considered (Figs. 22, 23).

Table 1. Material constants of the constitutive model (Section 3).

ρ_0 (kg/m^3)	C (J/kg·K)	E (MPa)	ν	α (K^{-1})	a (MPa)	b (MPa)
7800	500	200e+3	0.33	1e−6	0	15e+3

R_i (MPa)	R_{oo} (MPa)	k	$\gamma(°C^{-1})$	d_1	d_2	$\eta_2(MPa^{-2})(N=2)$
510	400	20	1.5e−3	0.05	0.05	0.01

Y (MPa·s$^{1/n}$)	n	Z (MPa·s$^{1/m}$)	m
100	10	10	2

Following simulations have been performed for $T_0 = 20°\text{C}$ and $\dot{\Gamma} = 1600\ \text{s}^{-1}$. The value of nominal shear strain at the damage incipience (strong deformation localization onset) is close to 39%.

Numerical strain components have been drawn versus the nominal shear strain Γ in Figs. 9 to 11. Strains have been obtained by integration from the corresponding expressions giving strain rates as follows:

$$(5.1)\qquad \begin{aligned} \dot{v}_{ij} &= d_{ij} + W_{ik}v_{kj} - v_{ip}W_{pj} \\ v_{ij}^{n+1} &= v_{ij}^{n} + \dot{v}_{ij}^{n+1}\cdot\Delta t \end{aligned} \qquad \text{where} \qquad \begin{aligned} v_{ij} &= \left(e_{ij}, e_{ij}^{e}, e_{ij}^{p}, e_{ij}^{d}\right), \\ d_{ij} &= \left(d_{ij}, d_{ij}^{e}, d_{ij}^{p}, d_{ij}^{d}\right). \end{aligned}$$

After the onset of damage, damage-related strain contribution increases while both elastic strain and plastic "regular" rate decrease: as the deformation concentrates more and more inside the bands, the mechanism of damage replaces progressively the mechanism of "regular" plasticity.

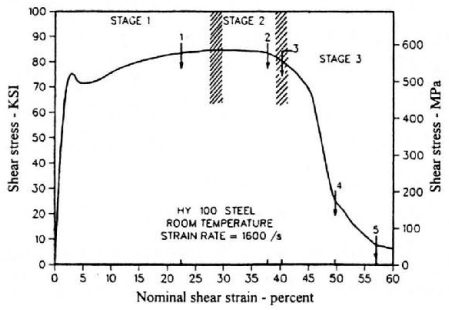

FIG. 7. Experimental stress-strain curve showing behaviour softening by ASB (after MARCHAND and DUFFY, [5]).

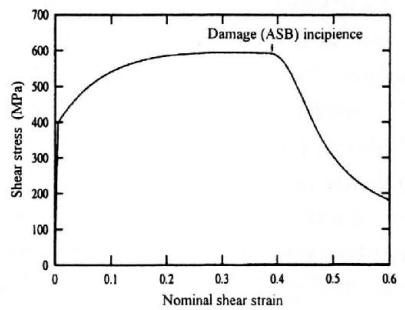

FIG. 8. Shear stress τ_{12} vs. nominal shear strain Γ reproduced by the 3D model.

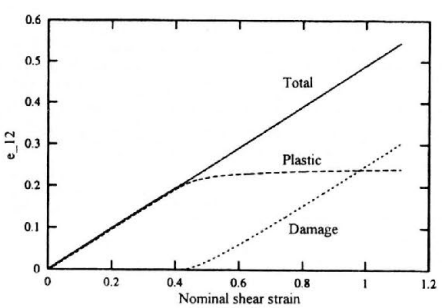

FIG. 9. Strain e_{12} vs. nominal shear strain Γ.

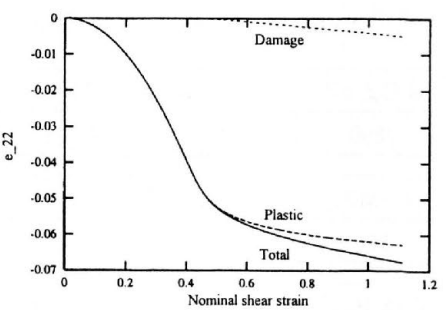

FIG. 10. Strain e_{22} vs. nominal shear strain Γ.

Numerical spin components have been drawn versus the nominal shear strain Γ in Fig. 12. According to (3.45), the rotation rate $\mathbf{W}$ represents, in the absence of damage, the spin $\boldsymbol{\omega}$ obtained from the anti-symmetric part of the velocity gradient $\mathbf{l}$. In this case, the objective derivative is simply the Zaremba-Jaumann derivative. After the onset of damage, Fig. 12 shows how the increase of damage-induced spin $\boldsymbol{\omega}^{\mathbf{d}}$ leads to the decrease of the rotation rate $\mathbf{W}$.

Total strain components have been drawn versus the nominal shear strain Γ in Fig. 13. After a value of nominal shear strain Γ close to 10%, strain components e_{11} and e_{22} increase and become significant compared with the strain e_{12}. This induces a change of the ratio e_{12}/Γ which is initially equal to 1/2. Finite rotation-related terms which appear in the time derivative $(5.1)_1$ are directly responsible for the existence of both strain components e_{11} and e_{22}. In the small deformation framework, these strain components would be zero because $(5.1)_1$ should be reduced to $v_{ij} = d_{ij}$. This remark concerns also time derivative of stress.

"Regular" temperature has been drawn versus the nominal shear strain Γ in Fig. 14. "Regular" temperature increases indeed until the damage onset. During the damage process, "regular" heating contribution decreases while "singular" heating contribution increases (see (3.32)) in relation to the damage variable growth.

Components of the thermo-elastic Kirchhoff stress tensor τ (called S_ij) have been drawn versus the nominal shear strain Γ in Fig. 15. The existence of stress components different from τ_{12} is a direct consequence of the finite deformation framework (see the remarks on strain derivatives). The various stress contributions to the generalized 2nd invariant $\hat{J}_2^s$ (called J_2) have been detailed in Fig. 16. It is noteworthy that, while the shear stress τ_{12} decreases strongly, the isotropic hardening conjugate force r remains significant. This preserves a certain strength of the material outside the bands.
The first invariant (density d) of the damage variable $\mathbf{D}$ has been drawn versus the nominal shear strain Γ in Fig. 17.

At the end of the calculations, the value of d is about 3. Interpretation of this result needs returning to the definition (2.2) of the density d of the damage variable $\mathbf{D}$:

$$d = d(T^*, ...).$$

In the case of simple shear, neglecting second order terms (resulting from complete time integration (5.1)), the thermo-elastic shear stress $(3.26)_1$ is approximately:

$$\tau_{12} = 2\mu e_{12}^e - 2b e_{12}^e \widetilde{D}_{22} = 2\left(\mu - b\widetilde{D}_{22}\right) e_{12}^e \tag{5.2}$$

where

$$\widetilde{D}_{22} = d\widetilde{n}_2\widetilde{n}_2, \qquad \widetilde{n} = (0,1,0). \tag{5.3}$$

According to (5.2) and (5.3), with the notation employed in (3.30), one can write:

$$C_{1212} = \mu - bd \tag{5.4}$$

where C_{1212} represents the current "global" shear modulus and μ is the initial shear modulus.

As shown in Fig. 18 below, the shear modulus can be approximated by a 2nd degree polynomial in temperature, in the interval [300 K, 1000 K]:

$$\mu(T) = \mu(0) - c_1 T - c_2 T^2 \qquad \text{with} \quad \begin{cases} c_1 = 8.1e-3 \text{ GPa/K}, \\ c_2 = 2e-5 \text{ GPa/K}^2. \end{cases} \tag{5.5}$$

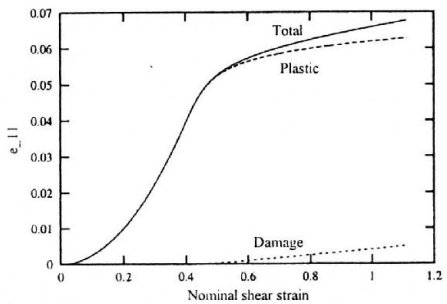

FIG. 11. Strain e_{11} vs. nominal shear strain Γ.

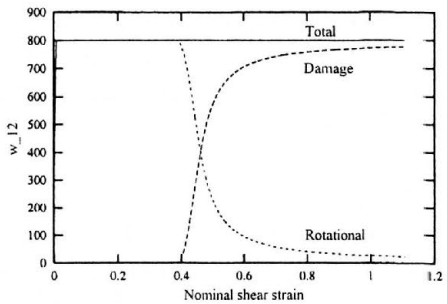

FIG. 12. Spin w_{12} vs. nominal shear strain Γ.

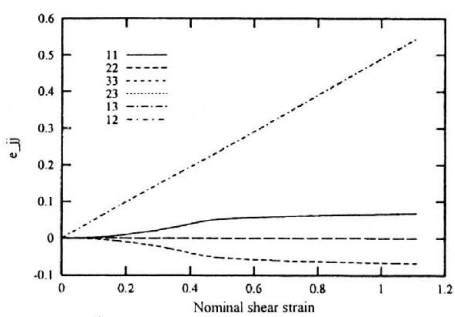

FIG. 13. Strains e_{ij} vs. nominal shear strain Γ.

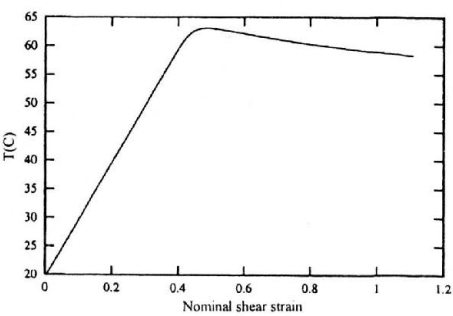

FIG. 14. "Regular" temperature vs. nominal shear strain Γ.

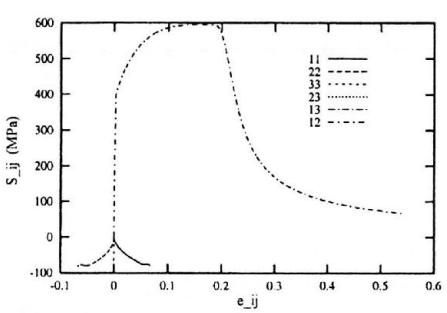

FIG. 15. Stress vs. nominal shear strain Γ.

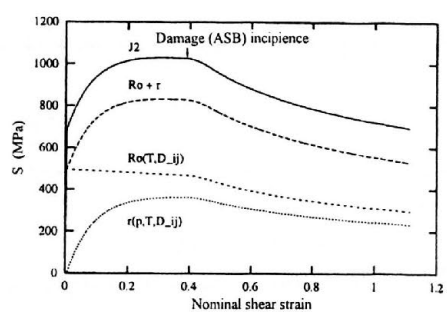

FIG. 16. $\hat{J}_2^s$ contributions vs. shear strain Γ.

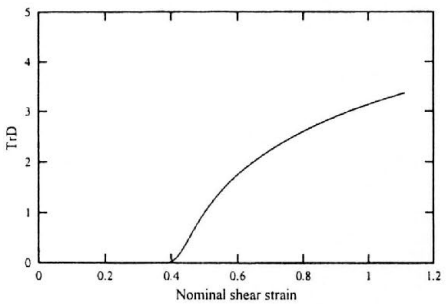

FIG. 17. Damage density vs. nominal shear strain Γ.

Fluctuations in shear modulus at low temperature (from 300 K to 400 K, which bound the range of "regular" temperature before the onset of damage) are weak, what justifies that the constitutive model supposes independence of the shear modulus μ from temperature in the elastic potential (3.15). On the other hand, at high temperature, especially inside the bands, the shear modulus is strongly affected. As the deformation is accommodated by ASB at advanced stage of localization, the current "global" shear modulus is close to the shear modulus of the band material.

Combining relations (5.4) from the present model with (5.5) yields:

$$\text{for } T > T_0^* \qquad C_{1212} = \mu(T^*) = \mu(0) - c_1 T^* - c_2 T^{*2} = \mu(T_0^*) - bd(T^*). \tag{5.6}$$

Rearranging (5.6) gives the following expression for $d(T^*)$:

$$d(T^*) = \frac{\mu(T_0^*) - \mu(0) + c_1 T^* + c_2 T^{*2}}{b}, \tag{5.7}$$

which verifies $d_{\min} = d(T_0^*) = 0$.

As a result of highly overestimating evaluation of an upper bound for $d = d(T^*)$, we can state first that temperature inside the band is bounded by the

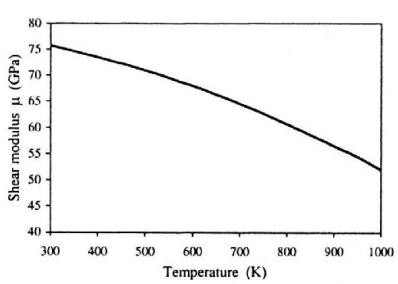

FIG. 18. Shear modulus μ vs. temperature for a hard steel (after JUANICOTENA [28] with $\mu(0) = 80$ GPa).

melting point. Consequently, the shear modulus is bounded by its value at the melting temperature. Extrapolating relation (5.5) to the melting temperature, the expression (5.7) gives the upper bound $d_{\max}$ of density d as:

$$d_{\max} = d(T_m) = \frac{\mu(T_0^*) - \mu(0) + c_1 T_m + c_2 T_m^{*2}}{b}. \tag{5.8}$$

If $\mu(T_m) \approx 0$, the upper bound $d_{\max}$ can be crudely approximated from (5.8) by:

$$d_{\max} \approx \frac{\mu}{b}. \tag{5.9}$$

The value of the material constant b, related to elastic energy degradation through the degradation of the shear stiffness produced by adiabatic shear banding, governs the upper bound $d_{\max}$. In the present numerical example, the value of b is chosen as 15 GPa (Table 1), which gives an upper bound for $d_{\max}$ close to 5. In the foregoing case (Fig. 17), the value close to 3 attained for nominal shear strain of about 1.2 is well below this limit. If prolonged further, the curve in Fig. 17 would ultimately approach (but never attain) the upper bound limit. Evolution of the current "global" shear modulus C_{1212} versus the nominal shear strain Γ is reported in Fig. 19.

In a tentative conclusion to this evaluation, it is interesting to note that when $b \to \mu$, then, according to (5.9), the interval of $d(T^*)$ is $[0, 1]$, and consequently, according to (5.4), the interval of C_{1212} is $[\mu, 0]$. In that interval, C_{1212} takes the values $\mu(1 - d(T^*))$ which can be approximated, following (5.7) and assuming independence of the shear modulus from temperature before damage incipience, by $\mu(0) - c_1 T^* - c_2 T^{*2}$. The shear stiffness of the representative volume becomes a function of the "singular" temperature only (with no b explicitly intervening). Fluctuations in "singular" temperature inside the band cluster are thus directly and exclusively responsible for fluctuations in the shear stiffness of the representative volume. This limiting case can be further explored in the fu-

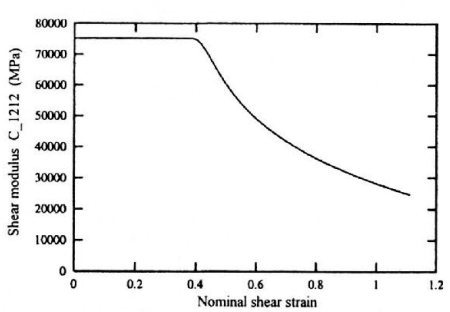

FIG. 19. Shear modulus C_{1212} vs. nominal shear strain Γ.

ture, especially in the context of mesh sensitivity control when performing finite element numerical calculations.

The upper bound of $d(T^*)$ being related to the value of shear degradation constant b (dependent on particular material) may represent some inconvenience in practical applications. Normalizing definitely the function $d(T^*)$ by fixing its maximum to, say e.g. 1, necessitates some technical modifications of the preceding equations (this will obviously shift in parallel the actual limit value of $d_{\max} = 1$ for $b \to \mu$). This subject will not be analysed here.

The components of the damage force tensor $\widetilde{\mathbf{k}}$ (called k_ij) have been drawn versus the 1st invariant (density) of the damage variable in Fig. 20 and versus the nominal shear strain Γ in Fig. 21. The damage conjugate force increases with the nominal shear strain. At the onset of damage, the component $\widetilde{k}_{22}$ diverges from $\widetilde{k}_{11}$ and $\widetilde{k}_{33}$ to increase more strongly in the damage process.

Different loading conditions have been imposed in shear to test the response of the model. Following effects have been illustrated in Figs. 22 and 23:

- nominal shear strain rate $\dot{\Gamma}$ effect on stress-nominal strain response;
- initial temperature T_0 effect on stress-nominal strain response.

Figure 22 shows that instability appears earlier when the nominal shear strain rate is higher. This agrees with the experimental investigations. Concurrently the influence of the nominal shear strain rate on stress increase is higher after the onset of damage.

Figure 23 shows that instability appears earlier when the initial temperature is lower. Numerical values of nominal shear strain Γ at the onset of localization do not agree exactly with experimental values obtained in [5]. The influence of the nominal shear strain rate on stress is higher before the onset of damage.

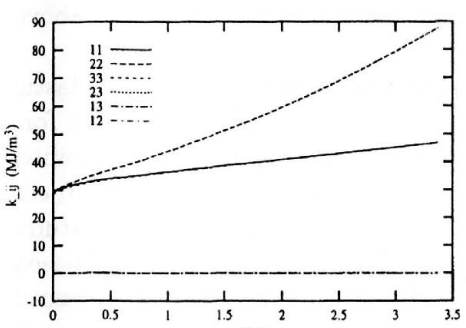

FIG. 20. Damage force $\widetilde{\mathbf{k}}$ vs. damage variable density d.

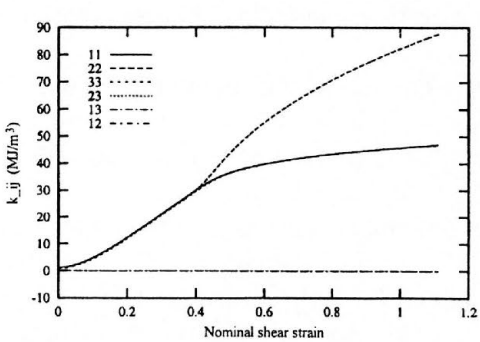

FIG. 21. Damage force $\widetilde{\mathbf{k}}$ vs. nominal shear strain Γ.

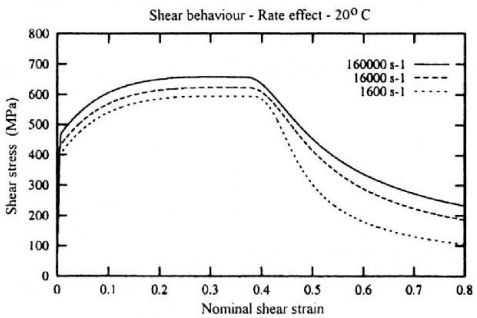

FIG. 22. Shear stress vs. nominal shear strain Γ, $T_0 = 20°$ C.

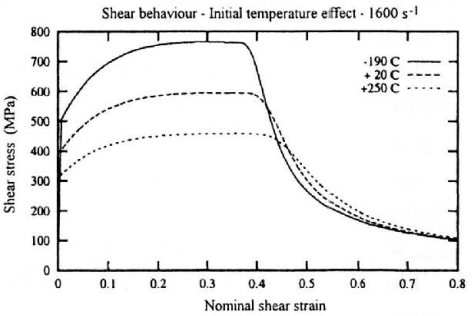

FIG. 23. Shear stress vs. nominal shear strain Γ, $\dot{\Gamma} = 1600\ \mathrm{s}^{-1}$.

6. Concluding remarks and perspectives

An elastic/viscoplastic constitutive model has been elaborated involving damage and damage-induced anisotropy produced by adiabatic shear banding. The latter deterioration mechanism has been captured through a second-order tensorial damage internal variable whose evolution is considered as rate-dependent (viscous) in some formal analogy to the plastic flow evolution.

As pointed out by PERZYNA *et al.* [11, 12], rate dependency favours maintaining ellipticity of the equations governing the evolution problem related to the class of constitutive models including the present one. The viscosity-related regularizing influence of the viscoplasticity and damage respective relaxation factors Y and Z (together with the exponents n and m; see Eqs. (3.39)–(3.40)) allows to overcome local instabilities, as it is shown in the numerical simulations above (Sect. 5).

The modelling methodology put forward herein in the finite elastic-plastic strain Eulerian framework has had to face the difficulties inherent for this formulation to cope with anisotropy effects and objectivity requirements combined [15]. As there is no clear consensus of the scientific community on this subject (while some convergent methodologies can be noticed, see e.g. LUBARDA's study [17] including damage and EKH and RUNESSON [16]), the Mandel-Sidoroff based approach has been favoured and adapted in this study. The analogy advanced here between an adiabatic shear band (ASB) cluster and a "super-dislocation" leads to a fairly simple evaluation of the damage-induced spin. The objective rotational derivatives can thus be operational within the model framework. By combining these specific factors, relevant to kinematics and anisotropy hypotheses, with thermodynamic postulates (existence of the free energy and dissipa-

tion potentials, and their consequences), a coherent model could be formulated. Some simplifying assumptions, regarding notably the strain hardening description and small elastic strain, have been made. The assumption of a single damage-plasticity yield function allows to express the strong coupling between the dissipative mechanisms at stake.

Constraints relative to consistent formulation of discretized boundary value problem and to relevant numerical implementation of the model have constituted a significant guideline to the formulation presented. Those aspects will be presented in details in forthcoming papers. Another question concerns the number and nature of material constants involved in the formulation presented. A compromise has been searched between conceptual pertinency of the constitutive model vs. complexity of mesomechanical and metallurgical phenomena and the tractability of the formalism advanced when applied to high velocity impact and penetration engineering problems. Those applications are currently under way.

Appendix A

$$C_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial e^e_{kl}} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - a\left(\delta_{ij}\widetilde{D}_{kl} + \widetilde{D}_{ij}\delta_{kl}\right) - b\left[\delta_{ik}\widetilde{D}_{jl} + \delta_{il}\widetilde{D}_{jk} + \widetilde{D}_{ik}\delta_{jl} + \widetilde{D}_{il}\delta_{jk}\right],$$

$$E_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial \widetilde{D}_{kl}} = -a\left[\delta_{ij}e^e_{kl} + \frac{e^e_{pp}}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\right] - b\left[e^e_{ik}\delta_{jl} + e^e_{il}\delta_{jk} + \delta_{ik}e^e_{jl} + \delta_{il}e^e_{jk}\right],$$

$$J_{ij} = \rho_0 \frac{\partial^2 \psi}{\partial e^e_{ij} \partial T} = -\alpha K \delta_{ij};$$

$$Q = \rho_0 \frac{\partial^2 \psi}{\partial p^2} = kR_\infty \exp(-kp)\exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right),$$

$$A_{ij} = \rho_0 \frac{\partial^2 \psi}{\partial p \partial \widetilde{D}_{ij}} = -R_\infty[1 - \exp(-kp)]\exp(-\gamma T) \cdot \exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right)\left[d_1\delta_{ij} + d_2\widetilde{D}_{ij}\right],$$

$$S = \rho_0 \frac{\partial^2 \psi}{\partial p \partial T} = -\gamma R_\infty[1 - \exp(-kp)]\exp(-\gamma T)\exp\left(-d_1\widetilde{D}_{kk} - \frac{d_2}{2}\widetilde{D}_{kl}\widetilde{D}_{lk}\right);$$

$$L_{ijkl} = \rho_0 \frac{\partial^2 \psi}{\partial \widetilde{D}_{ij} \partial \widetilde{D}_{kl}}$$
$$= +R_\infty \left[p + \frac{1}{k} \exp(-kp) \right] \exp(-\gamma T) \exp\left(-d_1 \widetilde{D}_{pp} - \frac{d_2}{2} \widetilde{D}_{mn} \widetilde{D}_{nm} \right)$$
$$\left\{ \left[d_1 \delta_{ij} + d_2 \widetilde{D}_{ij} \right] \left[d_1 \delta_{kl} + d_2 \widetilde{D}_{kl} \right] - \frac{d_2}{2} \left[\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right] \right\},$$

$$V_{ij} = \rho \frac{\partial^2 \psi}{\partial \widetilde{D}_{ij} \partial T} = \gamma R_\infty \left[p + \frac{1}{k} \exp(-kp) \right]$$
$$\cdot \exp(-\gamma T) \exp\left(-d_1 \widetilde{D}_{kk} - d_2 \widetilde{D}_{kl} \widetilde{D}_{lk} \right) \left[d_1 \delta_{ij} + d_2 \widetilde{D}_{ij} \right],$$

$$X = \rho_0 \frac{\partial^2 \psi}{\partial T^2}$$
$$= -\frac{\rho C}{T_0} + \gamma^2 R_\infty \left[p + \frac{1}{k} \exp(-kp) \right] \exp(-\gamma T) \exp\left(-d_1 \widetilde{D}_{kk} - d_2 \widetilde{D}_{kl} \widetilde{D}_{lk} \right).$$

Appendix B

$$Q^0 = \frac{\partial r}{\partial p} = k R_\infty \exp(-kp) \exp(-\gamma T),$$
$$S^0 = \frac{\partial r}{\partial T} = -\gamma R_\infty \left[1 - \exp(-kp) \right] \exp(-\gamma T),$$
$$G_{ijkl} = \frac{3}{2} \frac{\partial \left(\frac{s_{ij}}{J_2} \right)}{\partial \tau_{kl}} = \frac{3}{2 J_2} \left[I_{ijkl} - \frac{1}{3} \delta_{ij} \delta_{kl} - \frac{3}{2} \frac{s_{ij} s_{kl}}{J_2^2} \right];$$
$$P_{ij} = \frac{\partial \Lambda^p}{\partial \tau_{ij}} = \frac{\partial \Lambda^p}{\partial \mathcal{F}} \frac{\partial \mathcal{F}}{\partial \tau_{ij}} = \alpha K_{ij} = \frac{3}{2} \alpha \frac{s_{ij}}{J_2},$$
$$B = \frac{\partial \Lambda^p}{\partial p} = \frac{\partial \Lambda^p}{\partial \mathcal{F}} \frac{\partial \mathcal{F}}{\partial p} = -\alpha \frac{\partial r}{\partial p} = -\alpha Q^0,$$
$$E = \frac{\partial \Lambda^p}{\partial T} = \frac{\partial \Lambda^p}{\partial \mathcal{F}} \frac{\partial \mathcal{F}}{\partial T} = -\alpha \left(\frac{\partial R_0}{\partial T} + \frac{\partial r}{\partial T} \right) = -\alpha \left(\frac{\partial R_0}{\partial T} + S^0 \right);$$

$$\alpha = \frac{\partial \Lambda^p}{\partial \mathcal{F}} = n \frac{\dot{p}^{1 - \frac{1}{n}}}{Y}$$

$$EQ^0 = \frac{\partial \Lambda^p}{\partial T}\frac{\partial r}{\partial p} = -\alpha\left(\frac{\partial R_0}{\partial T} + S^0\right)Q^0$$

$$BS^0 = \frac{\partial \Lambda^p}{\partial p}\frac{\partial r}{\partial T} = -\alpha Q^0 S^0$$

$$\text{then} \quad \begin{cases} E + S^0\alpha = -\alpha\dfrac{\partial R_0}{\partial T} \\ EQ^0 - BS^0 = -\alpha\dfrac{\partial R_0}{\partial T}Q^0. \end{cases}$$

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Non-local coupling of viscoplasticity and anisotropic viscodamage for impact problems using the gradient theory

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Dedicated to Professor Piotr Perzyna on the occasion of his 70^{th} birthday

A GENERAL FRAMEWORK for the analysis of heterogeneous media that assesses a strong coupling between viscoplasticity and anisotropic viscodamage evolution is formulated for-impact related problems within the framework of thermodynamic laws and nonlinear continuum mechanics. The proposed formulations include thermo-elasto-viscoplasticity with anisotropic thermo–elasto–viscodamage, a dynamic yield criterion of a von Mises type and a dynamic viscodamage criterion, the associated flow rules, non-linear strain hardening, strain-rate hardening, and temperature softening. The constitutive equations for the damaged material are written according to the principle of strain energy equivalence between the virgin material and the damaged material. That is, the damaged material is modeled using the constitutive laws of the effective undamaged material in which the nominal stresses are replaced by the effective stresses. The evolution laws are impeded in a finite deformation framework based on the multiplicative decomposition of the deformation gradient into elastic, viscoplastic, and viscodamage parts. Since the material macroscopic thermomechanical response under high-impact loading is governed by different physical mechanisms on the macroscale level, the proposed three-dimensional kinematical model is introduced with manifold structure accounting for discontinuous fields of dislocation interactions (plastic hardening), and crack and void interactions (damage hardening). The non-local theory of viscoplasticity and viscodamage that incorporates macroscale interstate variables and their higher-order gradients is used here to describe the change in the internal structure and in order to investigate the size effect of statistical inhomogeneity of the evolution-related viscoplasticity and viscodamage hardening variables. The gradients are introduced here in the hardening internal state variables and are considered to be independent of their local counterparts. It also incorporates the thermomechanical coupling effects as well as the internal dissipative effects through the rate-type covariance constitutive structure with a finite set of internal state variables. The model presented in this paper can be considered as a framework, which enables one to derive various non-local and gradient viscoplasticity and viscodamage theories by introducing simplifying assumptions.

Key words: non-local theory; anisotropic viscodamage; viscoplasticity; gradient theory; heterogeneous media.

1. Introduction

THE INELASTIC MATERIAL behavior of engineering materials may be attributed to two distinct material mechanical processes: viscoplasticity (i.e. dislocations along crystal slip planes) and/or damage mechanics (cracks, voids nucleation and coalescense, decohesions, grain boundary cracks, and cleavage in the regions of high stress concentration). Plasticity/viscoplasticity theories, by themselves, are insufficient for modeling the material behavior since both damage defects (cracks and voids) and dislocation densities (viscoplastic flow) are present in their inelastic response. A constitutive model should address equally the two distinct physical modes of irreversible changes and should satisfy the basic postulates of mechanics and thermodynamics. A multi-dissipative model that accounts for both the material decohesions (discontinuities within a material) and the dislocations along slip planes is necessary. This is accomplished by adopting two loading surfaces and two potential functions, one for the viscoplasticity and another for the damage.

Experimental observations show that in general the processes of cold-working, forming, machining of mechanical parts, etc. can cause an initial evolution of defects in the virgin material state at localized zones, such as the nucleation of certain amount of cracks, voids, dislocation densities, and shear bands. Those localized defects of viscoplasticity (rate-dependent plasticity) and viscodamage (rate-dependent damage) induced in the material structure along with the subsequent defects that occur during deformation process lead to a heterogeneous (non-uniform) material behavior. Further loading of materials of this type will cause failure mechanisms to occur at localized zones of viscoplasticity and viscodamage. In those localized zones, a lot of defects may undergo irreversible growth; coalescence of pre-existing cracks and voids may occur; propagation of dislocations may proceed; and new defects may nucleate and their ultimate coalescence results in failure. Moreover, intensive interaction mechanisms of the evolved defects may take place at those localized zones; such as dislocation-dislocation interaction, microdamages-microdamages interaction, crack dominated-dislocation interaction, dislocation-dominated crack interaction, dislocation-crack grain boundary interaction, etc.

As the viscoplasticity and viscodamage defects localize over narrow regions of the continuum, the characteristic length-scale governing the variations of those defects and their average interactions over multiple length-scales falls far below the scale of the local state variables of viscoplasticity and viscodamage used to describe the response of the continuum. This leads to the loss of the statistical homogeneity in the representative volume element (RVE), in such a way that all the macroscopic response functions of interest (e.g. the Helmholtz free energy, Ψ; the dissipation potential, Π; the Cauchy stress tensor, $\boldsymbol{\sigma}$; the small strain tensor,

ε; the stiffness tensor; $\mathbf{C}$; etc.) are sensitive to the distribution, size, and orientation of the mesostructural and macrostructural defects within the RVE. The viscoplasticity and viscodamage evolution processes are, therefore, statistically inhomogeneous at the macroscale level (at the RVE scale). This suggests that the macroscopic inelastic deformations and failure are governed by mechanisms at different scale levels (nonlocality). For example, dislocation interactions are observed on a mesolevel with length-scale $0.1 - 10\mu$m GAO *et al* [36] affecting strongly the material behavior on the macrolevel with length-scale $\geq 100\mu$m. Thus, different methodologies rather than the local theories are necessary to adequately capture the decrease in the length-scale from the macroscale to the mesoscale level. The non-local theories are expanding steadily in order to appropriately overcome this problem, which take into account the influence of the n^{th} nearest neighbor of the material points or the long-range microstructural interaction.

Moreover, it is a well-known fact that the use of classical rate-independent plasticity theory or local theory do not possess an intrinsic length-scale, which leads to numerical stability problems, such as mesh size and mesh alignment sensitivities, particularly, in problems exhibiting strain localization phenomena. However, several regularization approaches have been proposed in the constitutive modeling to accommodate this problem. They include: viscoplastic models (e.g. PERZYNA [73], NEEDLEMAN [70], WANG *et al.* [106] DORNOWSKI and PERZYNA [30], GLEMA *et al.*, [43]), thermal dissipation models (e.g. LE MONDS and NEEDLEMAN [57], non-local models (e.g. AIFANTIS [2], PIJAUDIER-CABOT and BAZANT [85], BAZANT and PIJAUDIER-CABOT [14], VOYIADJIS and DELIKTAS [94], VOYIADJIS and DORGAN [97], and gradient models (AIFANTIS [3], ZBIB and AIFANTIS [107], DE BORST and SLUYS [27], FLECK and HUTCHINSON [35], BAMMANN *et al.*, [10], BUSSO *et al.* [19], VOYIADJIS *et al.* [96], BASSANI [11], GURTIN [44], VOYIADJIS and ABU AL-RUB [93]).

In the literature, many non-local plasticity/visco plasticity and damage/viscodamage models were proposed to introduce intrinsic length-scale measures in the constitutive equations, which can be grouped into two classes: integral models and gradient models.

KRÖNER [53] and ERINGEN and EDELEN [33] incorporated nonlocal terms through integral equations of elasticity. PIJAUDIER-CABOT and BAZANT [85], extended this concept to continuum damage mechanics. BAZANT and OZBOLT [13] also proposed a nonlocal anisotropic damage formulation, which is based on nonlocal tensorial variable. However, integration in the nonlocal integral models requires a global averaging procedure with resulting equations that can not be easily linearized (DE BORST and PAMIN [26]). This makes the nonlocal integral models computationally inefficient.

However, the integral approach generally involves an infinitely extended zone of nonlocal action and may be approxiamated by truncated Taylor series expansion, giving rise to the so-called gradient theories. Gradient approaches typically retain terms in the constitutive equations of higher-order gradients with coefficients representing length-scale measures of the deformation microstructure associated with the nonlocal continuum. AIFANTIS [2] was one of the first to study the gradient regularization in solid mechanics. The gradient methods suggested by LASRY and BELYTSCHKO [56] and MÜHLHAUS and AIFANTIS [69] provide an alternative approach to the nonlocal integral equations. The gradient terms in plasticity models are introduced through the yield function (e.g. MÜHLHAUS and AIFANTIS [69] DE BORST and MÜHLHAUS [25], DE BORST *et al.* [28], DE BORST and PAMIN [26], AIFANTIS *et al.* [4], GAO et al. [40], FLECK and HUTCHINSON [36], VOYIADJIS *et al.* [96]). The gradient damage theory has been developed for isotropic damage (e.g. PIJAUDIER-CABOT and BAZANT [85], PEERLINGS *et al.* [84], LACY *et al.* [55], GEERS *et al.* [42], SVEDBERG and RUNESSON [90], ZHOU *et al.* [111], ASKES and SLUYS [7]) and for anisotropic damage (e.g. KUHL *et al.* [54], VOYIADJIS and DELIKTAS [94], VOYIADJIS and DORGAN [97], VOYIADJIS and ABU AL-RUB [93]).

The motivation of this work comes from the experimental tests of specimens made of ductile materials and heterogeneous materials loaded at low- and high-speed impacts (BELINGARDI and VADORI [15], BORVIK *et al.* [18], LUO *et al.*, [64] ESPINOSA *et al.* [34], SIERAKOWSKI [87], ZHOU *et al.* [110], MONTAGNANI *et al.* [68], JOHNSON and COOK [47], ALBERTINI and MONTAGNANI [5] etc). Generally, these kinds of laboratory tests serve to verify the constitutive concepts and material parameters. In many of those tests, the intensive nonlinearity induced in the material is attributed to the viscoplasticity and viscodamage morphologies. Furthermore, the softening behavior in those experiments mostly appears as the result of temperature rise and damage growth. Those experiments indicate that the failure mechanisms occur at localized zones of viscoplasticity and viscodamage where a lot of interactions of defects take place. In order to be able to capture such localized deformation zones and strain-softening material behavior, we aim here to introduce explicit and implicit length-scale measures in plasticity and damage governing equations through the use of the gradient-dependent and viscoplasticity theories coupled to the viscodamage theory.

It is generally assumed that the rate of deformation can be additively decomposed into an elastic (reversible) part and an inelastic (irreversible) part (e.g. NEMAT-NASSER [75], LUBLINER [63], SIMO and HUGHES [89]). "Non-instantaneously reversible" deformation is a more general description of the inelastic deformation since it is corresponding to the following set of physical phenomena: instantaneous plasticity, viscoplasticity, instantaneous damage, and viscodamage. The first type of inelastic deformation is a time-independent mechanism,

which is generally considered in the rate-independent plasticity theories. The viscoplastic deformation, which is sometimes qualified as creep, is a rate-dependent mechanism. Both of those two mechanisms or one of them is generally not sufficient to describe the set of experimental observations under high strain rates (dynamic loadings). Therefore, degradation of the mechanical properties up to complete failure should be considered in the experimental simulations, in particular, simulating the heterogeneous material response under high strain-rates. This progressive physical process is commonly referred to as damage and it can be time-independent (damage theory) and/or time-dependent process (viscodamage theory). The evolution, nucleation, and coalescence of microcracks, voids, and cavities during manufacturing processes and subsequent loading enhance the material to behave inelastically in the elastic and plastic domains. VOYIADJIS and PARK [102] tend to sum such defects as an inelastic strain called the damage strain. They tend to decompose this damage strain into an elastic-damage (recoverable) component attributed to crack closure and void contraction during unloading, and an inelastic-damage (unrecoverable) component attributed to random distribution and orientation of the cracks that make their recovery impossible. Therefore, the second underlying motivation for this study is given by the work recently proposed by VOYIADJIS and PARK [102]. They presented a framework for finite nonlinear continuum damage involving seven different deformation configurations. In accordance with their work, two irreversible strains are considered in this study: the viscoplastic and viscodamage strains. The viscodamage strain component tends to be considerable in engineering materials under impact loading processes as compared to the viscoplastic strain component. We will also use a similar approach with a more attractive physical interpretation of the viscodamage deformation mechanisms. The proposed approach is analogous to the finite elasto-plasticity (e.g. NEMAT-NASSER [76], PERZYNA [82], LUBLINER [63], SIMO and HUGHES [89]) involving the multiplicative decomposition of the deformation gradient into elastic and inelastic parts. All configurations induced by the multiplicative decomposition are, as in finite elasto-plasticity, macroscopic. The damage evolution equations, however, are based on micromechanical considerations established through the use of gradient theory (for a detailed demonstration consult LACY *et al.* [55]).

There are many models with weak coupling between plasticity/viscoplasticity and damage/viscodamage; hence, no consistent model realizing a strong coupling has been published yet (HESEBECK [46]), which serves as our third motivation. In this work, the strong coupling between viscoplasticity and viscodamage will be implemented by using two independent viscodamage mechanisms. One mechanism is coupled with viscoplasticity, while the other one occurs independently of viscoplastic deformation. To formulate that on the basis of the thermodynamic principles, the two viscodamage processes are represented by two additive

portions in the dissipation potentials. Because this work focuses on the development of coupled viscoplastic-viscodamage governing equations based on thermomechanical postulates, the various possibilities to describe the viscoplasticity and anisotropic viscodamage will be considered here.

To mention some of the important contributions to phenomenological damage modeling, we have to start with effective stress concept of Kachanov (1958), who was the first to introduce for the isotropic case a one-dimensional variable, which may be interpreted as the effective surface density of microdamages per unit volume (VOYIADJIS and VENSON [104], VENSON and VOYIADJIS [91], VOYIADJIS *et al.* [105]). Following Kachanov's pioneering work researchers in different fields applied continuum damage mechanics to their areas in fields like brittle materials (KRAJCINOVIC and FONESKA [52], KRAJCINOVIC [51]) and ductile materials (e.g. LEMAITRE and CHABOCHE [59], LEMAITRE [60], KACHANOV [49], MURAKAMI [71]). In the 1990's coupling of continuum damage mechanics to plasticity have appeared (e.g. VOYIADJIS and VENSON [104], VOYIADJIS and KATTAN [98, 99, 100], LUBARDA and KRAJCINOVIC [62], VOYIADJIS and ABU-LEBDEH [92], VOYIADJIS *et al.* [105]).

The objective of this paper is to derive a general thermodynamic framework for the modeling of heterogeneous media that assess a strong coupling between viscoplasticity and viscodamage evolution for impact-related problems with considering the discontinuities on the macroscale level. The essential aspects of interest here can all be examined within the context of: (1) Finite strain kinematics; (2) Rapid time variations in temperature, strain, strain rate, and other field variables; (3) Viscodamage effects on moduli and strength (hardening/softening); (4) Strong viscoplasticity and viscodamage coupling; and (5) Numerical stability through using the regularization approaches (i.e., using viscoplasticity and viscodamage gradient-dependent theories). This can be effectively characterized through a thermodynamic framework for the development of a continuum thermo-elasto-viscodamage and thermo-elasto-viscoplastic based failure model. The constitutive equations are derived from the first and second laws of thermodynamics, the expression of Helmholtz free energy, the Clausius-Duhem inequality, the maximum dissipation principle, generalized normality, and the thermomechanical heat equation. All the thermodynamic equations are expressed in the spatial configuration. The evolution laws are impeded in a finite deformation framework based on the multiplicative decomposition of the deformation gradient and the additive decomposition of the spatial rate of deformation tensor into elastic, viscoplastic, and damage parts. The nonlocality is introduced here through the viscoplasticity and viscodamage hardening variables. The first-order gradients in the gradient-dependent theory are disregarded and the second-order gradients are mainly considered in this work. The local viscoplasticity and viscodamage hardening variables and their corresponding second-order gradients

are considered to be independent of each other, allowing one to computationally introduce independently the macroscale and mesoscale levels influence.

The outline of this paper is as follows: in Sec. 2, we outline a summary of the finite deformation kinematics and some of the fundamental definitions of nonlinear continuum mechanics. In Sec. 3, we outline a general thermodynamic framework for the elasto-viscoplastic and elasto-viscodamage material behavior with thermal effects for impact-related problems using the gradient-dependent theory. In Sec.4 the rate-type constitutive relation is derived. Finally, in Sec. 5 the thermomechanical couplings equation is formulated.

2. Finite deformation kinematics and fundamental definitions

2.1. Fundamental measure of total deformation

Here we summarize some of the fundamental definitions of nonlinear continuum mechanics (SIMO and HUGHES [80], BELYTSCHKO *et al.* [16], DOGHRI [29]) relevant to our subsequent developments. Our notation throughout is as follows: C^o and C^t are the manifolds, where we refer to a point $\mathbf{X} \in C^o$as a point in the reference configuration of a continuum body and a point $\mathbf{x} \in C^t$ as a point in the current configuration (at time t). Assuming that the deformation is smooth regardless of damage, one can assume a one-to-one mapping such that:

$$x_i = x_i(X, \mathrm{t}) \quad \text{or} \quad X_i = X_i(x, \mathrm{t}) \tag{2.1}$$

which maps the reference configuration C^o onto the spatial configuration C^t at time t. The corresponding deformation gradient is expressed as follows:

$$F_{ij} = \frac{\partial x_i}{\partial X_j} \tag{2.2}$$

which is a linear transformation for each $X \in C^o$ at time t.

Note that in this work the subscripts indicate the tensorial nature of the variables unless specifically stated otherwise.

For each $\mathbf{X} \in C^o$ there exists an orthogonal transformation $\mathbf{R}(\mathbf{X})$called rotation such that (polar decomposition):

$$F_{ij} = R_{ik}U_{kj} = V_{ik}R_{kj} \tag{2.3}$$

where $\mathbf{U}$ and $\mathbf{V}$ are the right and left stretch tensors, respectively.

The change in the squared length of a material filament $d\mathbf{X}$ is used as a measure of deformation such that for a Cartesian coordinate system:

$$\begin{aligned}(dl)^2 - (dL)^2 &= dx_i\, dx_i - dX_i\, dX_i, \\ &= 2E_{ij}dX_i\, dX_j,\end{aligned} \tag{2.4}$$

or

$$(dl)^2 - (dL)^2 = 2e_{ij}dx_i\,dx_j, \tag{2.5}$$

where $(dL)^2$ and $(dl)^2$ are the material filaments in the reference configuration C^o and the spatial configuration C^t, respectively. $\mathbf{E}$ and $\mathbf{e}$ are the material (or Lagrangian) and the spatial (or Eulerian) strain tensors, respectively, and are given by:

$$E_{ij} = \frac{1}{2}\left(F_{ki}F_{kj} - \delta_{ij}\right) = \frac{1}{2}\left(C_{ij} - \delta_{ij}\right) \tag{2.6}$$

and

$$e_{ij} = \frac{1}{2}\left(\delta_{ij} - F_{ki}^{-1}F_{kj}^{-1}\right) = \frac{1}{2}\left(\delta_{ij} - c_{ij}\right), \tag{2.7}$$

where $\mathbf{C} = \mathbf{U}^2$ and $\mathbf{b} = \mathbf{c}^{-1} = \mathbf{V}^2$ are the right and left Cauchy-Green tensors, respectively, and δ_{ij} is the Kronecker delta. $\mathbf{C}$ is defined with respect to the reference configuration while $\mathbf{b}$ is with respect to the current configuration.

For the spatial strain tensor $\mathbf{e}$ and the material strain tensor $\mathbf{E}$ we have:

$$e_{ij} = F_{ki}^{-1}E_{kl}F_{lj}^{-1}. \tag{2.8}$$

The spatial velocity, denoted by $\boldsymbol{\upsilon}(\mathbf{x}, t)$, is the time derivative of the motion:

$$\upsilon_i = \frac{\partial x_i}{\partial t}. \tag{2.9}$$

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

$$l_{ij} = \frac{\partial \upsilon_i}{\partial x_j} = \dot{F}_{ik}F_{kj}^{-1}. \tag{2.10}$$

where the dot denotes the time derivative. The symmetric part of $\mathbf{l}$, denoted by $\mathbf{d}$, is called the spatial rate of deformation tensor, and its skew-symmetric part is called the spin (or vorticity) tensor, $\boldsymbol{\omega}$. Thus one obtains:

$$d_{ij} = \frac{1}{2}\left(l_{ij} + l_{ji}\right) \tag{2.11}$$

and

$$\omega_{ij} = \frac{1}{2}\left(l_{ij} - l_{ji}\right). \tag{2.12}$$

Let us define the Lagrangian rate of deformation tensor **D** and the Eulerian rate of deformation tensor **d** as follows:

$$D_{ij} = \dot{E}_{ij} = \frac{1}{2}\dot{C}_{ij}, \tag{2.13}$$

$$d_{ij} = \frac{1}{2}F^{-1}_{ki}\dot{C}_{kl}F^{-1}_{lj}. \tag{2.14}$$

Utilizing Eq. (2.13) into Eq. (2.14), d is then related to D by:

$$d_{ij} = F^{-1}_{ki}D_{kl}F^{-1}_{lj}. \tag{2.15}$$

while the spatial deformation rate tensor **d** is equal to the Cotter-Rivin convected rate of the Eulerian (Almansi) strain tensor as follows:

$$d_{ij} = L_v(e_{ij}) = \dot{e}_{ij} + e_{ik}l_{kj} + e_{kj}l_{ki} \tag{2.16}$$

where the symbol L_ν denotes the well-known Lie derivative with respect to $\boldsymbol{\nu}$ (MARSDEN and HUGHES, [67]).

2.2 Rates of the stress tensors

The first Piola-Kirchhoff stress tensor **P** is a nonsymmetric nominal stress tensor obtained by performing a Piola transformation on the Cauchy stress tensor $\boldsymbol{\sigma}$, i.e.

$$P_{ij} = JF^{-1}_{ik}\boldsymbol{\sigma}_{kj} \tag{2.17}$$

where J denotes the Jacobian of the deformation and represents the ratio of the mass densities at the reference configuration and the current configuration:

$$J = \frac{\rho^o}{\rho} = \frac{dv}{dV} = \det(\mathbf{F}), \tag{2.18}$$

where ρ^o and ρ are the mass densities of the reference and current configurations, respectively. dV and dv are the initial volume and the volume after deformation, respectively.

The symmetric (or second) Piola-Kirchhoff stress tensor **S** is defined as follows:

$$S_{ij} = F^{-1}_{ik}P_{kj} = JF^{-1}_{ik}\boldsymbol{\sigma}_{kl}F^{-1}_{jl} = F^{-1}_{ik}\tau_{kl}F^{-1}_{jl} \tag{2.19}$$

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

The rate of the Kirchhoff stress tensor (the Lie derivative) is given as follows:

$$L_v(\tau_{ij}) = F_{ik}\dot{S}_{kl}F_{jl} = \dot{\tau}_{ij} - l_{ik}\tau_{kj} - l_{jk}\tau_{ik} \tag{2.20}$$

where $\dot{\boldsymbol{\tau}}$ defines the material time derivative of the Kirchhoff stress tensor which is given by the following relation:

$$\dot{\tau}_{ij} = \frac{\partial \tau_{ij}}{\partial t} + \frac{\tau_{ij}}{\partial x_k} v_k \tag{2.21}$$

The Jaumann-Zaremba stress rate of the Kirchhoff stress is defined as follows:

$$\tau^o_{ij} = \dot{\tau}_{ij} - \omega_{ik}\tau_{kj} + \omega_{kj}\tau_{ik} \tag{2.22}$$

Using Eqs. (2.11) and (2.12) along with Eq. (2.22), we can express the Jaumann-Zaremba stress rate, $\boldsymbol{\tau}^o$, in terms of the Lie derivative of the Kirchhoff stress tensor ($L_v\boldsymbol{\tau}$) and the spatial rate of deformation (d) as follows:

$$\tau^o_{ij} = L_v(\tau_{ij}) + d_{ik}\tau_{kj} + d_{kj}\tau_{ik}. \tag{2.23}$$

Note that both the first and second Piola-Kirchhoff stress tensors, $\mathbf{P}$ and $\mathbf{S}$, are relevant to the reference configuration C^o, while the Kirchhoff and Cauchy stress tensors, $\boldsymbol{\tau}$ and $\boldsymbol{\sigma}$, are relevant to the current configuration C^t. Also note that the elastic components of the rate of deformation (d) and the spin tensor ($\boldsymbol{\omega}$) should be substituted in the stress rate tensors $L_v\boldsymbol{\tau}$ and $\boldsymbol{\tau}^o$.

2.3. The deformation rate additive decomposition

Imagine an elastically loaded representative volume element (RVE) containing uniformly distributed (micro)-cracks of Mode I, which are triggered by the process of cold working, is deformed by a total strain ε_1. A certain part of this strain will be elastically recoverable (ε_1^e) and another part can be induced by damage (ε_1^{ed}). When the loads are released before yield limit, the body will have no permanent strains left. However, the elastic stiffness of the RVE could have been reduced by the growth of microcracks. This is clearly demonstrated in Figure 1 which shows the foregoing micromechanics of a continuum point in the RVE and the corresponding macro-stresses and strains.

Imagine now the elastically loaded RVE containing an arbitrary distribution of (micro)-voids and (micro)-cracks of mixed modes (Mode I, II, and III), which are triggered by the process of cold working, and subjected to 3-D state of stress. Generally, this situation is more likely to happen in materials than the above one. This RVE is deformed by a total strain of $\boldsymbol{\varepsilon}$ a certain part of it will be elastically recoverable ($\boldsymbol{\varepsilon}^e$) and another part is induced by damage ($\boldsymbol{\varepsilon}^d$). When the loads are released before the yield limit, the body will have, similarly to plasticity and

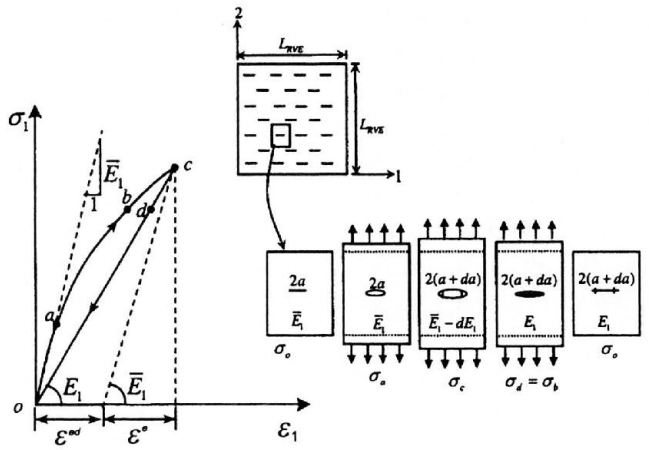

FIG. 1. Fictitious uniaxial stress-strain elastic response resulting from a growing micro-crack. All damage strain is recoverable (the crack is closed but not healed).

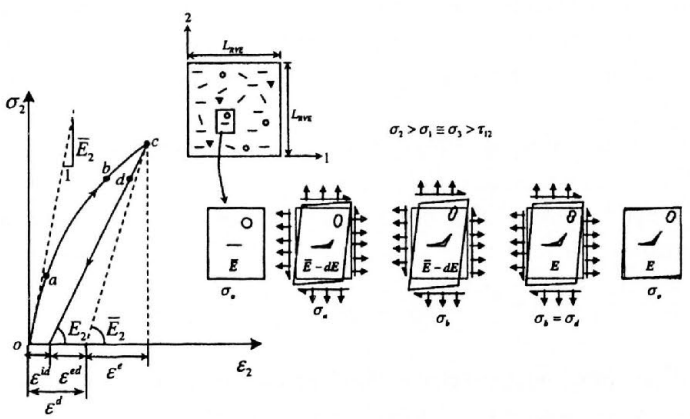

FIG. 2. Fictitious stress-strain elastic response of an RVE subjected to 3-D state of stress $\sigma_2 > \sigma_1 \cong \sigma_3 > \tau_{12}$ resulting from a growing microcrack and microvoid. Part of the damage strain is recoverable (not healed) and the other part is unrecoverable.

in contrast to the above fictitious situation, permanent deformations left ($\boldsymbol{\varepsilon}^{id}$). Fig. 2 shows the underlying micromechanics of a continuum point in the RVE and the corresponding macro-stresses and strains in one of the directions.

Motivated by the above discussion and assuming small elastic and finite viscoplastic and viscodamage deformations under high-impact loading, we can postulate the additive decomposition of the total spatial deformation rate tensor ($\mathbf{d}$) into elastic ($\mathbf{d}^e$), viscoplastic ($\mathbf{d}^{vp}$), and viscodamage components ($\mathbf{d}^d$). Although

the damage process is an irreversible deformation thermodynamically; however, the deformation due to damage itself can be partially or completely recovered upon unloading. Thus, the damage deformation component is also decomposed into elastic-damage (reversible) and viscoinelastic-damage (irreversible) parts. The recoverable part is attributed to crack closure upon unloading (but not healing), while the unrecoverable part is attributed to the lack of crack closure and void contraction that cause permanent deformation. Both cause degradation in the material stiffness (ABU AL-RUB and VOYIADJIS [1]). Hence, the total deformation rate tensor can be written as:

$$d_{ij} = d^e_{ij} + d^{vp}_{ij} + d^d_{ij} \tag{2.24}$$

and

$$d^d_{ij} = d^{ed}_{ij} + d^{id}_{ij}, \tag{2.25}$$

where $\mathbf{d}^{ed}$ and $\mathbf{d}^{id}$ are the elastic-damage and viscoinelastic-damage parts of the damage strain, respectively. The superscripts here do not imply tensorial indices but merely indicate the corresponding deformation configuration such as "e" for elastic, "vp" for viscoplastic, "d" for damage, "ed" for elastic-damage, and "id" for inelastic-damage.

During the unloading process, two types of deformation rates are purely reversible: the ordinary elastic deformation rate $\mathbf{d}^e$ and the elastic-damage deformation rate $\mathbf{d}^{ed}$. Thus, the total reversible elastic deformation rate $\mathbf{d}^E$ upon unloading can be obtained by:

$$d^E_{ij} = d^e_{ij} + d^{ed}_{ij}. \tag{2.26}$$

On the other hand, the total viscoinelastic rate of deformation d^I arises from the two irreversible sources: viscoinelastic damage and viscoplastic flow, such that:

$$d^I_{ij} = d^{id}_{ij} + d^p_{ij}, \tag{2.27}$$

hence Eq. (2.24) can be rewritten as:

$$d_{ij} = d^E_{ij} + d^I_{ij}. \tag{2.28}$$

The viscoinelastic damage may occur during only elastic deformations (in the absence of plastic deformations) under the condition that micro-cracks occur without the presence of a plastic process zone ahead of the crack tip.

Many researchers tend to adopt the traditional simple isotropic scalar damage variable, "$(1-\phi)$", to model the material micro-damage mechanism, in which

all components of the material stiffness are degraded by the same scalar damage parameter, ϕ. However, to ensure a more realistic application of the principles of the damage mechanics, anisotropic damage will be assumed. In this case different levels of damage are related to the principal directions, and thus a simple scalar damage parameter is no longer sufficient to quantify damage in all directions. Instead, the anisotropic phenomenon of the microcracks distribution in the material is interpreted using a symmetric second-order damage tensor, ϕ_{ij}.

The linear elastic constitutive equations for the damaged material are written according to the principle of elastic strain energy equivalence between the virgin material and the damaged material (SIDOROFF, [86]). That is, the damaged material is modeled using the constitutive laws of the effective undamaged material in which the Kirchhoff stress tensor τ is replaced by the effective stress tensor $\bar{\boldsymbol{\tau}}$ (MURAKAMI and OHNO, [70]):

$$\bar{\boldsymbol{\tau}}_{ij} = \mathbf{M}_{ikjl}\boldsymbol{\tau}_{kl} \tag{2.29}$$

where $\mathbf{M}$ is the fourth order damage-effect tensor. Many different expressions for $\mathbf{M}$ exist in the literature. A comprehensive review of the most widely used expressions are presented by VOYIADJIS and PARK [101]. The following expression for $\mathbf{M}$, which have been proposed by CORDEBOIS and SIDOROFF [24], is used here due to its attractiveness in the mathematical formulations and its symmetrization ability of the effective stress tensor $\bar{\boldsymbol{\tau}}$, such that:

$$\mathbf{M}_{ikjl} = 2\left[\left(\delta_{ik} - \phi_{ik}\right)\delta_{jl} + \delta_{ik}\left(\delta_{jl} - \phi_{jl}\right)\right]^{-1} \tag{2.30}$$

where δ_{ij} is the Kronecker delta.

The elastic-damage stiffness $\mathbf{C}$ in the case of finite deformation is given by VOYIADJIS and PARK [102] as follows:

$$C_{ijkl} = N_{ikjl}\bar{C}_{klpq}N_{prqs} \tag{2.31}$$

where

$$\begin{aligned} N_{ikjl} &= M^{-1}_{ikjl} \\ &= a_{ik}a_{jl} = \tfrac{1}{2}\left[\left(\delta_{ik} - \phi_{ik}\right)\delta_{jl} + \delta_{ik}\left(\delta_{jl} - \phi_{jl}\right)\right] \end{aligned} \tag{2.32}$$

and $\bar{\mathbf{C}}$ is the fourth-order elastic moduli tensor given by:

$$\bar{C}_{ijkl} = K\delta_{ij}\delta_{kl} + 2G\left(\delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{ij}\delta_{kl}\right), \tag{2.33}$$

where K is the bulk modulus and G is the shear-modulus in the effective configuration.

The rate of the Kirchhoff stress tensor is defined in terms of the elastic deformation tensor as follows:

$$L_v(\tau_{ij}) = \bar{\Im}_{ijkl} d^e_{kl} \tag{2.34}$$

where $\bar{\Im}$ is the effective spatial elasticity tensor related to the effective fourth-order tensor of elastic constants $\bar{\mathbf{C}}$ by the (push-forward) transformation as follows:

$$\bar{\Im}_{ijkl} = F_{ir} F_{js} F_{km} F_{ln} \bar{C}_{rsmn}. \tag{2.35}$$

Similarly, Eqs. (2.34) and (2.35) can be defined using the Jaumann-Zaremba stress rate tensor as follows:

$$\tau^o_{ij} = \bar{a}_{ijkl} d^e_{kl}\,. \tag{2.36}$$

where

$$\bar{a}_{ijkl} = \bar{\Im}_{ijkl} + \delta_{il}\tau_{jk} + \delta_{jl}\tau_{ik}\,. \tag{2.37}$$

2.4. Finite elasto-viscoplastic and elasto-viscodamage deformations

The processes of cold-working, forming, machining of mechanical parts, etc. can leave an initial damage. The initial damage induced in the material microstructure along with the subsequent damage that occurs during elastic loading, enhance the material to behave inelastically before viscoplasticity occurs. Therefore, if the material is elastically unloaded before forming dislocations along slip planes (viscoplasticity), permanent strains consist observed. Those strains are irreversible damage strains, while the reversible damage strains consist of two parts: elastic part and damage part. Then, if viscoplasticity occurs, both viscodamage and viscoplastic permanent deformations are anticipated.

First we motivated this basic behavior in one dimension. Consider the uniaxial tension test shown in Fig. 3. In this test, a bar of uniform cross-section is subjected to the uniaxial loading history: $O \to B \to C$, during which the length of the bar takes the following values: $L \to l^{vp} \to l^{pid} \to l^{vpd} \to l$. Stage $O \to B$ corresponds to a monotonic loading beyond the elasticity domain, and $B \to C$ to elastic-damage unloading ($C \to B$ corresponds to elastic-damage loading process). State C corresponds to a stress-free, unloaded configuration. We can write the following trivial identity:

$$\frac{l}{L} = \frac{l}{l^{vpd}} \frac{l^{vpd}}{l^{vp}} \frac{l^{vp}}{L} \tag{2.38}$$

or

$$\lambda = \lambda^e \lambda^d \lambda^{vp}, \tag{2.39}$$

where $\lambda = l/L$ is the axial stretch at the end of $O \to B$, $\lambda^e = l/l^{vpd}$ can be viewed as the elastic stretch at the end of the elastic transformation $B \to F$, $\lambda^d = l^{vpd}/l^{vp}$ corresponds to the viscodamage stretch between D state and a viscodamage-free state between C and O, and $\lambda^{vp} = l^{vp}/L$ corresponds to viscoplastic stretch between O state and a viscoplastic-free state between C and O. Additionally, λ^d can be written as:

$$\frac{l^{vpd}}{l^{vp}} = \frac{l^{vpd}}{l^{vpid}} \frac{l^{vpid}}{l^{vp}} \tag{2.40}$$

or

$$\lambda^d = \lambda^{ed}\lambda^{id}, \tag{2.41}$$

where $\lambda^{ed} = l^{vpd}/l^{vpid}$ is the elastic-damage stretch (recoverable viscodamage stretch) between states $D \to C$, and $\lambda^{id} = l^{vpid}/l^{vp}$ is the unrecoverable viscodamage stretch between C state and a viscodamage-free state between C and O.

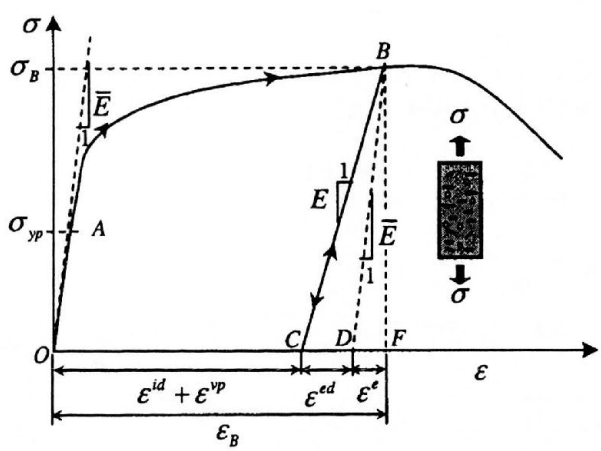

FIG. 3. Uniaxial stress-strain response of a metallic specimen.

The illustration of Fig. 4 in three dimensions is similar to that of the one-dimensional case (Fig. 3). If O designates the initial state (C^o), B the current state (C^t), and $D \to O$ (C^{dvp}, C^{vpid}, and C^{vp}) the local intermediate, stress-free, unloaded states, then the deformation gradients are: $\mathbf{F}$ for $O \to B$, $\mathbf{F}^e$ for $D \to B$, $\mathbf{F}^d$ between D state and a viscodamage-free state $D \to O$, and $\mathbf{F}^{vp}$ between state O and a viscoplastic-free state between O and C. Additionally, $\mathbf{F}^d$ can be decomposed into $\mathbf{F}^{ed}$ for $C \to B$, $\mathbf{F}^{id}$ between C state and a viscodamage-

free state between $C \to O$. Thus, the deformation gradient $\mathbf{F}(X,t)$ is split into elastic, viscoplastic, and viscodamage parts as follows:

$$\frac{\partial x}{\partial X} = \frac{\partial x}{\partial x^{vpd}} \frac{\partial x^{vpd}}{\partial x^{vp}} \frac{\partial x^{vp}}{\partial X} \tag{2.42}$$

or

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^{vp} \cdot \mathbf{F}^d, \tag{2.43}$$

introducing tacitly the local intermediate natural state configurations. In the sequel we suppose that elastic strains are small compared to viscoplastic and viscodamage strains. Also $\mathbf{F}^d$ is split into elastic-damage (reversible) part and inelastic-viscodamage (irreversible) part as:

$$\frac{\partial x^{vpd}}{\partial x^{vp}} = \frac{\partial x^{vpd}}{\partial x^{vpid}} \frac{\partial x^{vpid}}{\partial x^{vp}} \tag{2.44}$$

or

$$\mathbf{F}^d = \mathbf{F}^{ed} \cdot {}^{id} \tag{2.45}$$

Therefore, the total deformation gradient can be decomposed into total elastic part ($\mathbf{F}^E = \mathbf{F}^e . \mathbf{F}^{ed}$) and inelastic part ($\mathbf{F}^I = \mathbf{F}^{id} . \mathbf{F}^{vp}$), such that:

$$\mathbf{F} = \mathbf{F}^E . \mathbf{F}^I . \tag{2.46}$$

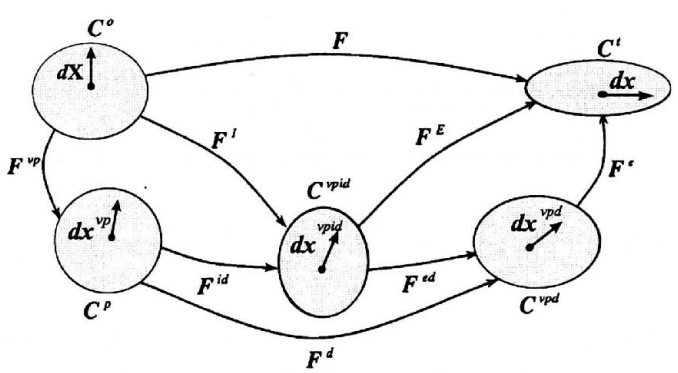

FIG. 4. Illustration of the multiplication decomposition of the deformation gradient.

The determinate of the total deformation tensor J (or the Jacobian of deformation, Eq. (2.18)) that characterizes the volumetric deformation can then be

multiplicatively decomposed into elastic, viscoplastic, and viscodamage parts as follows:

$$J = J^e J^{vp} J^d \tag{2.47}$$

where

$$J^e = \det(\mathbf{F}^e); \quad J^{vp} = \det(\mathbf{F}^{vp}); \quad J^d = \det\left(\mathbf{F}^d\right) \tag{2.48}$$

3. Constitutive modeling for dynamic impact loading

3.1. Thermodynamic formulation

In this section, the thermo-elasto-viscoplastic and thermo-elasto-viscodamage material behavior is considered. This means that the strain, strain rate, temperature material dependence, and the nonlinear material response are considered. The dependent constitutive variables are functions of the Eulerian total elastic strain tensor ($\mathbf{e}^E$), temperature (T), temperature gradient (∇T), the deformation gradient tensor ($\mathbf{F}$), the measure of volumetric deformation ($J = \det(F)$), and n_{int}- of phenomenological internal state variables ($\aleph_k$, $k = 1, ..., n_{int}$; $n_{int} \geq 1$). Hence, within the thermodynamic framework the thermoelastic Helmholtz free energy density at the current state of deformation can be written as (DUSZEK-PERZYNA and PERZYNA, [32]):

$$\Psi = \tilde{\Psi}\left(e^E_{ij}, T, \nabla_i T, F_{ij}, J; \aleph_k\right). \tag{3.1}$$

However, by considering the assumption of small elastic strains (usually accepted for metals and other materials subjected to high strain-rate loading), the specific free energy function Ψ may be written as follows (MURNAGAHAM [37], GARCIA GARINO and OLIVER [41] CELENTANO [21]):

$$\Psi = \tilde{\Psi}\left(e^E_{ij}, T, \nabla_i T, J; \aleph_k\right) \tag{3.2}$$

Moreover, under severe loading conditions the elastic strains are comparably smaller. Thus, the elastic part of the deformation gradient can be assumed to be unity (i.e., $J^e = I$). By adopting, also, the incompressibility assumption (i.e., $J^p = I$), which is an acceptable postulate for metals, we can rewrite the specific free energy function Ψ as follows:

$$\Psi = \tilde{\Psi}\left(e^E_{ij}, T, \nabla_i T, J^d; \aleph_k\right) \tag{3.3}$$

where $J^d = \det(\mathbf{F}^d)$. This last simplified form of Ψ is used in the formulation described below.

Analogous to the additive decomposition of the deformation rate d^E into elastic and elastic-damage components (Eq. (2.26)), the Eulerian total elastic strain tensor e^E can be also decomposed as follows:

$$e_{ij}^E = e_{ij}^e + e_{ij}^{ed}. \tag{3.4}$$

This additive decomposition of the Almansi total elastic strain can also be deduced from the multiplicative decomposition of the deformation gradient into elastic and elastic-damage parts, $\mathbf{F}^E = \mathbf{F}^e . \mathbf{F}^{ed}$.

Since the main objective is to develop the rate-type constitutive equations for a viscoplastic and viscodamage material, the effects of viscoplastic strain hardening/softening, viscodamage strain hardening/softening, micro-damage mechanism, and thermomechanical coupling have to be considered. In order to compensate for such mechanisms, a finite set of internal state variables $\aleph_k$ $(k = 1, ..., n_{int})$ representing either scalars or tensorial variables are assumed, such that:

$$\aleph_k = \tilde{\aleph}_k \left(\phi_{ij}, \Xi_n, \nabla^2 \Xi_n\right) \tag{3.5}$$

where $\boldsymbol{\phi}$ is the average damage density, Ξ_n $(n = 1-4)$ are the viscoplasticity and viscodamage hardening variables, and $\nabla^2 \Xi_n$ are the corresponding higher-order gradients (Laplacian) of Ξ_n.

We make use here of the postulate of the isotropic influence of averaging of the evolution equations of the assumed internal state variables Ξ_n over a representative volume element (RVE). The first-order gradients are disregarded and the second-order gradients are mainly considered in this work. Moreover, setting Ξ_n and $\nabla^2 \Xi_n$ as independent internal state variables allows one to computationally introduce independently the macro and meso-scales. It also allows these two different physical phenomena to be identified separately with different evolution equations. This approach is considered in this paper. The set of the macro internal variables Ξ_n is postulated as follows:

$$\Xi_n = \tilde{\Xi}_n \left(p, \alpha_{ij}, r, \Gamma_{ij}\right) \tag{3.6}$$

where p denotes the accumulative or equivalent viscoplastic strain and α denotes the flux of the residual stress (backstress). p is associated with the isotropic hardening and α with the kinematic hardening in the viscoplastic flow process. Similarly, r denotes the accumulative viscodamage and Γ denotes the flux of the residual stress (kinematic hardening) in the damage flow process. Those viscoplasticity and viscodamage hardening variables are introduced in the Helmholtz free energy density in order to provide sufficient details of the deformation defects (cracks, voids, mobile and immobile dislocation densities) and their interactions in order to properly (i.e. physically) characterize the material microstructure behavior. These variables will provide an adequate characterization of these defects

in terms of size, orientation, distribution, spacing, interaction among defects, and so forth. In addition, in order to be able to achieve this, macroscale discontinuities influence should to be addressed and implemented properly.

For the strain-softening regime of the material behavior, the non-homogenous states of deformation can appear as localized regions with large deformations. A suitable description of the evolution of such zones can be obtained with the use of a non-local or gradient theory, examples of which are given by AIFANTIS [2], MÜHLHAUS and AIFANTIS [69], BAZANT *et al.* [12], and VOYIADJIS *et al* [96]. The gradient theory introduces in the material constitutive equations higher-order deformation gradients with coefficients that represent length-scale measures that characterize microstructural links with the non-local continuum. An attempt is made here to account for the non-uniform macroscale viscodamage and viscoplastic distribution on the overall macroscale response by assuming the thermoelastic Helmholtz free energy density Ψ to depend not only on the macroscopic response associated with the internal variables Ξ_n, but also on its macroscopic spatial higher-order gradients $\nabla^2\Xi_n$. Both Ξ_n and $\nabla^2\Xi_n$ are considered to be independent of each other. This postulate is motivated through the fact that certain internal state variables such as the mobile and immobile dislocation densities do not necessarily have the same evolution equations (BAMMANN and AIFANTIS, [8, 9]). They have different physical interpretations that guide one to different evolution equations for Ξ_n and $\nabla^2\Xi_n$. Thus, the set of internal state variables $\nabla^2\Xi_n$ are postulated as follows:

$$\nabla^2\Xi_n = \nabla^2\tilde{\Xi}_n\left(\nabla^2 p, \nabla^2\alpha_{ij}, \nabla^2 r, \nabla^2\Gamma_{ij}\right) \tag{3.7}$$

where $\nabla^2(\square)$ denotes the corresponding higher-order gradient Laplacian of $(\square)$. The assumed dependence of the Helmholtz free energy on the distinct variables $\nabla^2\Xi_n$ is also motivated by the necessity to include length-scale measures into the equations of state that link the mesoscale interactions to the macroscale viscoplasticity and viscodamage, which can not be captured by Xi_n variables only.

The viscoplastic hardening presented by the internal state variables p and α accounts for the dislocation interactions. The isotropic hardening internal state variables p and $\nabla^2 p$ are associated with the density of dislocations in the current state and characterized by statistically stored dislocations and geometrically necessary dislocations, respectively (GAO *et al.*, [40] FLECK and HUTCHINSON, [36]). The kinematic hardening variables α and $\nabla^2\alpha$ correspond to the incompatibility of viscoplastic deformation between various parts of the material (LEMAITRE and CHABOCHE,[59]). Hence, the viscoplasticity hardening variables depend on the interaction of the statistically stored or mobile dislocations and geometrical necessary or immobile dislocation densities. On the other hand, the viscodamage

hardening presented by the internal state variables r and Γ accounts for retardation of the (micro)-crack growth at higher strain rates resulting from (micro)-crack growth arrested by other (micro)-defects (VOYIADJIS and DELIKTAS, [95], ABU AL-RUB and VOYIADJIS, [1]). The gradient of the assumed internal state variable is used to describe the corresponding non-local material behavior, i.e. it is used to overcome the deficiency of the classical continua to capture the length-scale effects due to localization of viscoplasticity and viscodamage. The damage variable ϕ reflects the material degradation at a micromechanical scale due to nucleation and coalescence of voids, cavities, and microcracks in an averaged sense. The determination of the assumed internal state variables is the main challenge of the constitutive modeling.

The proposed viscoplastic and viscodamage constitutive modeling is formulated within the framework of thermodynamic principles; that is, the use of balancing laws, the conservation of mass, linear and angular momenta, and the first and second laws of thermodynamics. Those fundamental laws of continuum mechanics in the spatial representation can be written as follows (COLEMAN and GURTIN [23], LUBLINER [63], LEMAITRE and CHABOCHE [59], BELYTSCHKO *et al.* [16], DOGHRI [29]):

(i) Conservation of mass

$$\dot{\rho} + \rho div\,(v_i) = 0 \quad \text{or} \quad \rho J = \rho^o. \tag{3.8}$$

(ii) Balance of linear momentum

$$div\left(\frac{1}{J}\tau_{ij}\right) + \rho b_i = \rho \dot{v}_i. \tag{3.9}$$

(iii) Balance of moment of momentum

$$\tau_{ij} = \tau_{ji}. \tag{3.10}$$

(iv) Conservation of energy (first law of the thermodynamics)

$$\dot{u} = \frac{1}{\rho^o}\tau_{ij}d_{ij} + h - \frac{1}{\rho}q_{k,k}. \tag{3.11}$$

(v) Law of entropy (second law of the thermodynamics)

$$\rho\dot{\eta} + div\left(\frac{q_i}{T}\right) - \rho\frac{h}{T} \geq 0. \tag{3.12}$$

and the Clausius-Duhem inequality, which can be derived from the previous laws of thermodynamics, such that:

$$-\dot{u} + \dot{\eta}T + \frac{1}{\rho^o}\tau_{ij}d_{ij} - \frac{q_i}{\rho T}\nabla_i T \geq 0 \tag{3.13}$$

where ρ^o is the reference mass density, ρ is the current mass density, v is the spatial velocity vector, b is the specific body force vector, u is the internal energy density, h is the external specific heat source, η is the specific (per unit mass) entropy, q is the heat flux vector, and $J > 0$ is the determinate of the deformation gradient tensor $\mathbf{F}$. ∇ denotes the first order gradient ($\nabla_i = \partial/\partial x_i$). Meanwhile, u, Ψ, T, and η are related by:

$$\Psi = u - T\eta \tag{3.14}$$

Using the above equation in Eq. (3.13), one can rewrite the Clausius-Duhem inequality as follows:

$$\tau_{ij}d_{ij} - \rho^o\left(\dot{\Psi} + \eta\dot{T}\right) - J\frac{q_i}{T}\nabla_i T \geq 0. \tag{3.15}$$

Note that the time rate of a spatial field ($\dot{f}$) is defined as the material-time derivative (Df/Dt) and given as follows:

$$\dot{f} = \frac{Df}{Dt} = \frac{\partial f}{\partial t} + v_m\frac{\partial f}{\partial x_m}. \tag{3.16}$$

The Lie derivative of Eq. (3.3) with respect to its internal state variables in the updated configuration is given by:

$$\dot{\psi} = \frac{\partial \psi}{\partial e^E_{ij}}d^E_{ij} + \frac{\partial \psi}{\partial T}\dot{T} + \frac{\partial \psi}{\partial \nabla_i T}\overline{\nabla_i T} + \frac{\partial \psi}{\partial J^d}\dot{J}^d + \frac{\partial \psi}{\partial \aleph_k}L_v(\aleph_k) \tag{3.17}$$

where

$$\frac{\partial \Psi}{\partial \aleph_k}L_v(\aleph_k) = \frac{\partial \Psi}{\partial \phi_{ij}}L_v(\phi_{ij}) + \frac{\partial \Psi}{\partial \Xi_n}L_v(\Xi_n) + \frac{\partial \Psi}{\partial \nabla^2\Xi_n}L_v(\nabla^2\Xi_n). \tag{3.18}$$

The last two terms of Eq. (3.18) are given by:

$$\frac{\partial \Psi}{\partial \Xi_n}L_v(\Xi_n) = \frac{\partial \Psi}{\partial p}\dot{p} + \frac{\partial \Psi}{\partial \alpha_{ij}}L_v(\alpha_{ij}) + \frac{\partial \Psi}{\partial r}\dot{r} + \frac{\partial \Psi}{\partial \Gamma_{ij}}L_v(\Gamma_{ij}). \tag{3.19}$$

and

$$\frac{\partial \Psi}{\partial \nabla^2\Xi_n}L_v(\nabla^2\Xi_n) = \frac{\partial \Psi}{\partial \nabla^2 p}\overline{\nabla^2 p} + \frac{\partial \Psi}{\partial \nabla^2\alpha_{ij}}L_v(\nabla^2\alpha_{ij}) + \frac{\partial \Psi}{\partial \nabla^2 r}\overline{\nabla^2 r} + \frac{\partial \Psi}{\partial \nabla^2\Gamma_{ij}}L_v(\nabla^2\Gamma_{ij}). \tag{3.20}$$

Note that in Eq. (3.17) the Lie derivative of the Almansi total elastic strain ($L_v e^E$) defines the total elastic spatial rate of deformation tensor (d^E). The material-time derivative of the Jacobian of the damage deformation ($\dot{J}^d$) is expressed as follows:

$$\dot{J}^d = \frac{\partial J^d}{\partial F^d_{ij}} \dot{F}^d_{ij} = J^d d^d_{ij} \delta_{ij}. \tag{3.21}$$

Substituting the rate of the Helmholtz free energy density (Eq. (3.17)) into the Clausius-Duhem inequality (Eq. (3.15)), one obtains:

$$\begin{aligned} &\left(\tau_{ij} - \rho^o \frac{\partial \psi}{\partial e^E_{ij}}\right) d^e_{ij} \\ &\quad + \left(\tau_{ij} - \rho^o \frac{\partial \psi}{\partial e^E_{ij}} - \rho^o \frac{\partial \psi}{\partial J^d} J^d \delta_{ij}\right) d^{ed}_{ij} + \left(\tau_{ij} - \rho^o \frac{\partial \psi}{\partial J^d} J^d \delta_{ij}\right) d^{id}_{ij} \\ &+ \tau_{ij} d^{vp}_{ij} - \rho^o \left(\frac{\partial \psi}{\partial T} + \eta\right) \dot{T} - \rho^o \frac{\partial \psi}{\partial \nabla_i T} \overline{\nabla_i T} - \rho^o \frac{\partial \psi}{\partial \aleph_k} L_v \aleph_k - J \frac{q_i}{T} \nabla_i T \geq 0. \end{aligned} \tag{3.22}$$

Assume that the axiom of entropy production holds, then the above inequality equation results in the following thermodynamic state laws:

$$\begin{aligned} &\tau_{ij} = \rho^o \frac{\partial \psi}{\partial e^E_{ij}}; \quad \eta = -\frac{\partial \psi}{\partial T}; \quad \frac{q_i}{\dot{T}} = \rho^o \frac{\partial \psi}{\partial \nabla_i T}; \\ &P = -\rho^o \frac{\partial \psi}{\partial J^d}; \quad \sum_k = \rho^o \frac{\partial \psi}{\partial \aleph_k}. \end{aligned} \tag{3.23}$$

The above equations describe the relation between the state variables (observable and internal) and their associated thermodynamic conjugate forces. These thermodynamic forces conjugate to their state variables are listed in Table 1, where $\Sigma_k = \{Y, R, X, K, H, R^g, X^g, K^g, H^g\}$ are the conjugate forces corresponding to the viscoplastic and viscodamage internal variables $\Xi_k = \{\phi, p, \boldsymbol{\alpha}, r, \Gamma, \nabla^2 p, \nabla^2 \boldsymbol{\alpha}, \nabla^2 r, \nabla^2 \Gamma\}$,respectively. The stress τ is a measure of the elastic changes in the internal structure, while $\mathbf{Y}$ is a measure of the elastic-damage changes in the internal structure resulting from crack closure and void contraction during the unloading process. The conjugate forces R and $\mathbf{X}$ are measures of the viscoplastic changes in the internal structure, while K and $\mathbf{H}$ are measures of the viscoinelastic-damage changes in the internal structure. P is the thermodynamic pressure, where Eq. $(3.23)_4$ is consistent with the definition of thermodynamic tension (which is opposite in sign to that of pressure) of Gibbsian thermodynamics (NARASIMHAN [73]).

Table 1. Thermodynamic state variables and their corresponding conjugate forces.

State Variables		Associated Conjugates
Observable	Internal	
e		τ
T		η
	e^E	τ
	e^I	$-\tau$
	J^d	P
	∇T	q
	$p, \quad \nabla^2 p$	$R, \quad R^g$
	$\alpha, \quad \nabla^2 \alpha$	$X, \quad X^g$
	$r, \quad \nabla^2 r$	$K, \quad K^g$
	$\Gamma, \quad \nabla^2 \Gamma$	H, $\quad H^g$
	ϕ	Y

The additive decomposition of the rate of deformation tensor (Eq. (2.24)) implies that the Helmholtz free energy function Ψ can be written as a sum of elastic, viscoplastic, and viscodamage portions, such that:

$$\Psi\left(e_{ij}^E, T, \nabla_i T, J^d; \aleph_k\right) = \Psi^e\left(e_{ij}^E, T, \nabla_i T, \phi_{ij}\right) + \Psi^{vp}\left(T, \nabla_i T, p, \nabla^2 p, \alpha_{ij}, \nabla^2 \alpha_{ij}\right) + \Psi^d\left(T, \nabla_i T, J^d, r, \nabla^2 r, \Gamma_{ij}, \nabla^2 \Gamma_{ij}, \phi_{ij}\right) \tag{3.24}$$

where Ψ^e is the thermoelastic stored energy, while $\Psi^{vp}$and Ψ^d are the energy stored due to material hardening.

The complexity of a model is directly determined by the form of the Helmholtz free energy Ψ and by the number of conjugate pairs of variables. It is possible to decouple the Helmholtz free energy into a potential function of each internal state variable in such a way that an analytical expression for the thermodynamic potential is given as a quadratic form of its internal state variables. However, coupling is possible in the viscoplastic potential or the viscodamage potential if they depend on more than one variable (HENRY and HASLACH [45]), which makes the evolution equations more complex. CHABOCHE [22] said that an energy Ψ with non-quadratic kinematic hardening variables leads to abnormal results, but coupling with temperature was not discussed there. In high velocity impact-related problems, very high-strain rates combined with large deformations can produce a significant temperature rise due to adiabatic heating, where most of the work done on solids is usually dissipated in the form of heat resulting in local increase

in temperature, which affects the behavior of the material during deformation. This necessitates the inclusion of the temperature in the constitutive modeling of the material. KAPOOR and NEMAT-NASSER [50] measured the energy converted to heat during inelastic flow using infra-red method for some metal alloys. The infra-red measurements showed that 70% of the work done is converted to heat. BJERKE *et al.* [17] examined experimentally the role of plastic deformation in generating heat during dynamic compression and fracture of polycarbonate, where Split Hopkinson pressure bar (SHPB) experiments and opening mode dynamic mode fracture experiments were performed to measure the thermomechanical response of polycarbonate at various loading conditions. The results indicate that plastic deformation is not the main source of heat generation during the dynamic fracture, but it only accounts for about 8% of the measured heating and the other portion is due to thermofracture coupling providing that the deformation is the only source of material heating. Hence, the thermomechanical coupling in both viscoplasticity and viscodamage mechanisms needs to be considered in the material behavior modeling for more accurate comparisons with the experiments. A necessary explicit multiplicative temperature coupling term can be introduced in the hardening state variables for more realistic description of their evolution equations and good conformity with the experimental observations that show strong dependence of such states on temperature.

The thermoelastic energy (Ψ^e) is postulated as follows:

$$\Psi^e = \frac{1}{2\rho^0} e^E_{ij} \Im_{ijkl}(\phi)\, e^E_{kl} - \frac{1}{\rho^0}\beta_{ij} e^E_{ij}\Delta T - \eta_r \Delta T - \frac{1}{2} c \Delta T^2 - \frac{1}{2\rho^0 \dot{T}} k_{ij} \nabla_i T \nabla_j T \tag{3.25}$$

and the viscoplastic and viscodamage energies, Ψ^{vp} and Ψ^d, on the long term manifolds (neglecting the short term manifolds) are respectively assumed to have the following analytical forms, such that:

$$\Psi^{vp} = \frac{\vartheta}{2\rho^o}\left[a_1 p^2 + a_2\left(\nabla^2 p\right)^2 + a_3 \alpha_{ij}\alpha_{ij} + a_4 \nabla^2 \alpha_{ij} \nabla^2 \alpha_{ij}\right] \tag{3.26}$$

$$\Psi^d = \frac{\vartheta}{2\rho^o}\left[a_5 r^2 + a_6\left(\nabla^2 r\right)^2 + a_7 \Gamma_{ij}\Gamma_{ij} + a_8 \nabla^2 \Gamma_{ij} \nabla^2 \Gamma_{ij}\right] + c_v\left(T^{ig} - T_r\right) \tag{3.27}$$

where $\Im(\boldsymbol{\phi})$ is the fourth-order damage elastic tensor and is a function of $\boldsymbol{\phi}$, $\boldsymbol{\beta}$ are the thermo-mechanical coefficients, c is the coefficient of thermal expansion,

η_r is the reference entropy, $a_k (k = 1 - 8)$ are the material-dependent constants, $\mathbf{k}$ is the heat conductivity coefficients tensors, $\Delta T = T - T_r$ is the temperature difference, ϑ is the homologous temperature defined as $\vartheta = 1 - (T/T_m)^n$, where n is the temperature softening component, T_r is the reference temperature, and T_m is the melting temperature. c_v is the specific heat at constant volume (or the constant volume heat capacity), and T^{ig} is chosen to have the form of ideal gas temperature that can be expressed as follows:

$$T^{ig} = T_r \exp\left[(\eta - \eta_r)/c_v\right] \left[1 + \varepsilon^d\right]^{(\gamma-1)} \exp\left[(\gamma - 1)\left(1 \Big/ \left(1 + \varepsilon^d\right) - 1\right)\right]. \tag{3.28}$$

$\gamma = c_p/c_v$ is the ratio of the specific heats, where c_p is the specific heat at constant pressure. Both c_v and c_p are related to the gas constant $\Re$ by $\Re = c_p - c_v$. The above expression is postulated in order to derive an expression for the equation of state, which relates pressure to specific density. ε^d is the nominal volumetric damage strain, which can be expressed in terms of J^d as:

$$\varepsilon^d = \frac{1}{J^d} - 1. \tag{3.29}$$

Note that in this paper the foregoing material properties are taken as independent of temperature unless specifically stated otherwise.

The proposed definition of Ψ allows the derivation of the constitutive equations and the internal dissipation described next. Moreover, the definition of the different contributions of Ψ given by Eqs. (3.25), (3.26), and (3.27) consider the density at the initial configuration ρ^o instead of its current value ρ. This simplification is consistent with most of the large strain models exists in the literature (see DOYLE and ERICKSEN [31], DUSZEK-PERZYNA and PERZYNA [32], CELENTANO [21] etc). However, any density change in the evolution equations is given by the conservation of mass law (Eq. (56)). The constitutive equations for stress and entropy, Eqs. $(3.23)_1$ and $(3.23)_2$, can be written from the thermodynamic potential equations, Eqs. (3.25), (3.26), and (3.27), by neglecting higher-order derivatives, such that:

$$\tau_{ij} = \Im_{ijkl} e^E_{kl} - \beta_{ij} \Delta T, \tag{3.30}$$

where

$$\Im_{ijkl} = \rho^o \frac{\partial^2 \Psi}{\partial e^E_{ij} \partial e^E_{kl}} \quad , \quad \beta_{ij} = -\rho^o \frac{\partial^2 \Psi}{\partial e^E_{ij} \partial T}, \tag{3.31}$$

and

$$\eta = \eta_e + \eta_{vp} + \eta_d, \tag{3.32}$$

where

$$\eta_e = \eta_r + c\Delta T + \frac{1}{\rho^o}\beta_{ij}e^E_{ij}, \tag{3.33}$$

$$\eta_{vp} = \frac{1}{2\rho^o}\left[a_1 p^2 + a_2\left(\nabla^2 p\right)^2 + a_3\alpha_{ij}\alpha_{ij} + a_4\nabla^2\alpha_{ij}\nabla^2\alpha_{ij}\right]\frac{\partial\vartheta}{\partial T} \tag{3.34}$$

$$\eta_d = \frac{1}{2\rho^o}\left[b_1 r^2 + b_2\left(\nabla^2 r\right)^2 + b_3\Gamma_{ij}\Gamma_{ij} + b_4\nabla^2\Gamma_{ij}\nabla^2\Gamma_{ij}\right]\frac{\partial\vartheta}{\partial T} \tag{3.35}$$

with

$$\frac{\partial\vartheta}{\partial T} = \frac{n}{T_m}\left(\frac{T}{T_m}\right)^{n-1}. \tag{3.36}$$

In Eq. (3.30) the instantaneous elasticity tensor $\mathfrak{F}$ could be considered constant either on the spatial (updated) or in the material (reference) configuration. If it is considered constant in the material configuration, $\mathfrak{F}$ is obtained by "push forward" operation, while if it is considered constant on the spatial configuration, the elasticity tensor in the material configuration comes out by performing a "pull back" operation (CAR *et. al.* [20]).

The constitutive equations for the heat flux vector $\mathbf{q}$ and the pressure stress P can be obtained from Eqs. $(3.23)_3$ and $(3.23)_4$, respectively, as follows:

$$\mathbf{q}_i = -k_{ij}\nabla_j T \tag{3.37}$$

which is the Fourier heat conduction equation. The negative sign indicates that the heat flow is opposite to the direction of temperature increase.

The thermodynamic pressure stress P is given as follows:

$$P = (1-\gamma)\, c_v T^{ig}\varepsilon^d \tag{3.38}$$

which gives the equation of state necessary for high-impact loading. The equation of state accounts for compressibility effects (changes in density) and irreversible thermodynamic processes.

Coupling between elasticity and damage does exist indirectly since the elastic modulus is a function of the damage variable $\boldsymbol{\phi}$. Furthermore, coupling between viscoplasticity and viscodamage exists since the viscoplastic thermodynamic states are expressed in the current damaged configuration. The state laws of the assumed internal state variables, Eq. $(3.23)_5$, are obtained from Table 1 and the thermodynamic potential equations Eqs. (3.25), (3.26), and (3.27) are

expressed in Table 2 in terms of their associated internal state variables. The superscript 'g' in Table 2 indicates the thermodynamic conjugate force corresponding to the gradient internal variable. Other choices of the Helmholtz free energy function Ψ lead to conjugate forces which differ in algebraic form but not in the fundamental concept from the specific case considered here.

Table 2. The thermodynamic conjugate forces.

Plasticity	Isotropic Hardening	$R = \rho^o \frac{\partial \Psi^{vp}}{\partial p} = a_1 p\vartheta$, $R^g = \rho^o \frac{\partial \Psi^{vp}}{\partial \nabla^2 p} = a_2 \left(\nabla^2 p\right)\vartheta$
	Kinematic Hardening	$X_{ij} = \rho^o \frac{\partial \Psi^{vp}}{\partial \alpha_{ij}} = a_3 \alpha_{ij}\vartheta$, $X^g_{ij} = \rho^o \frac{\partial \Psi^{vp}}{\partial \nabla^2 \alpha_{ij}} = a_4 \left(\nabla^2 \alpha_{ij}\right)\vartheta$
Damage	Isotropic Hardening	$K = \rho^o \frac{\partial \Psi^d}{\partial r} = b_1 r\vartheta$, $K^g = \rho^o \frac{\partial \Psi^d}{\partial \nabla^2 r} = b_2 \left(\nabla^2 r\right)\vartheta$
	Kinematic Hardening	$H_{ij} = \rho^o \frac{\partial \Psi^d}{\partial \Gamma_{ij}} = b_3 \Gamma_{ij}\vartheta$, $H^g_{ij} = \rho^o \frac{\partial \Psi^d}{\partial \nabla^2 \Gamma_{ij}} = b_4 \left(\nabla^2 \Gamma_{ij}\right)\vartheta$
	Damage Force	$-Y_{ij} = \rho^o \frac{\partial \Psi^e}{\partial \phi_{ij}} = \frac{\partial}{\partial \phi_{ij}} \left[\frac{1}{2} e^E_{ij} \Im_{ijkl}(\phi)\, e^E_{kl}\right]$

Substituting of Eqs. (3.23) into Eq. (3.22) modifies the Clausius-Duhem inequality to express the fact that dissipation energy Π is necessarily positive, such that:

$$\Pi = \tau_{ij} d^I_{ij} + P J^d d^d_{ij} \delta_{ij} - \Pi_{int} - q_i \left[\frac{\dot{\overline{\nabla_i T}}}{\dot{T}} + J \frac{\nabla_i T}{T}\right] \geq 0 \tag{3.39}$$

where the rate of internal dissipation Π_{int} is given by the relation:

$$\Pi_{int} = \sum_k L_v \aleph_k = -R\dot{p} - R^g \dot{\overline{\nabla^2 p}} - X_{ij} L_v(\alpha_{ij}) - X^g_{ij} L_v(\nabla^2 \alpha_{ij}) \tag{3.40}$$

$$- K\dot{r} - K^g \dot{\overline{\nabla^2 r}} - H_{ij} L_v(\Gamma_{ij}) - H^g_{ij} L_v(\nabla^2 \Gamma_{ij}) + Y_{ij} L_v(\phi_{ij}) \geq 0.$$

Based on the previous assumption of Helmholtz free energy additive decomposition (Eq. (3.24)), the dissipation energy (Eq. (3.39)) can be rewritten as the summation of dissipation energies due to mechanical dissipation (viscoplasticity and viscodamage) and thermal dissipation, such that:

$$\Pi = \Pi^{vp} + \Pi^d + \Pi^{th} \geq 0, \tag{3.41}$$

where

$$\Pi^{vp} = \tau_{ij} d^{vp}_{ij} - R\dot{p} - R^g \overline{\nabla^2 p} - X_{ij} L_v(\alpha_{ij}) - X^g_{ij} L_v(\nabla^2 \alpha_{ij}) \geq 0, \tag{3.42}$$

$$\Pi^{d} = \tau_{ij} d^{id}_{ij} + P J^d d^d_{ij} \delta_{ij} - K\dot{r} - K^g \overline{\nabla^2 r} - H_{ij} L_v(\Gamma_{ij}) - H^g_{ij} L_v(\nabla^2 \Gamma_{ij}) + Y_{ij} L_v(\phi_{ij}) \geq 0, \tag{3.43}$$

$$\Pi^{th} = -q_i \left[\frac{\overline{\nabla_i T}}{\dot{T}} + J \frac{\nabla_i T}{T} \right] \geq 0. \tag{3.44}$$

This result requires that all inelastic work should dissipate away as heat, except for that energy which is stored because of the rearrangement of the material internal structure. Note that not dissipation occurs not only due to deviatoric stresses associated with d^{vp} and $\mathbf{d}^{id}$ but also due to the pressure stress associated with $\mathbf{d}^d$. This result suggests that viscoinelastic-damage deformation is controlled by deviatoric as well as volumetric stresses, while the elastic-damage deformation is mainly controlled by volumetric stresses. Moreover, writing the dissipation potential function Π as in the decoupled form shown in Eq. (3.41) does not mean that the corresponding physical mechanisms are decoupled. Coupling does occur in the viscoplastic potential given by Eq. (3.42) between viscoplasticity and viscodamage since the conjugate forces are expressed in the current deformed and damaged configuration of the material. Hence, two additive damage mechanisms are introduced in the dissipation function (Eq. (3.41)); one mechanism is coupled with viscoplasticity and the other occurs independently of viscoplastic deformation. Complementary laws can be related to the dissipation processes given by Eqs. (3.42) and (3.43). This implies the existence of the dissipation potential expressed as a continuous and convex scalar-valued function of the flux variables.

It is obvious that the definition of Ψ and consequently of $L_v \aleph_k$ $(k = 1 - 9)$ are essential features of the thermodynamic formulation in order to describe the thermomechanical/microstructural behavior of the material involved in the deformation process. The evolution laws of $\mathbf{d}^I$ and $\boldsymbol{\phi}$ can be obtained by utilizing the calculus of several variables with Lagrange multipliers $\dot{\Lambda}^{vp}$ and $\dot{\Lambda}^d$. The dissipation function $\Pi^I = \Pi^{vp} + \Pi^d$ (Eq. (3.41)) is subjected to the two constraints, namely $f = 0$ and $g = 0$ (VOYIADJIS and KATTAN [98]), such that:

$$\Omega = \Pi^{vp} + \Pi^d - \dot{\Lambda}^{vp} f - \dot{\Lambda}^d g. \tag{3.45}$$

For generality purposes, we will assume here that the time-dependent behavior of both viscoplasticity and viscodamage mechanisms are controlled by different relaxation times associated with $\dot{\Lambda}^{vp}$ and $\dot{\Lambda}^{d}$, which may not generally be the case. This congruous is suggested to occur only for material impact behavior above a certain material threshold of impact speed. This is not the subject of the present work, but it will be discussed thoroughly in a forthcoming paper.

Now we make use of the maximum viscoinelastic dissipation principle (SIMO and HONEIN [88], SIMO and HUGHES [89]), which states that the actual state of the thermodynamic forces ($\boldsymbol{\tau}$, $\mathbf{Y}$) is that which maximizes the viscoinelastic dissipation function over all other possible admissible states. Thus, we maximize the objective function Ω by using the necessary conditions as follows:

$$\frac{\partial \Omega}{\partial \tau_{ij}} = 0 \quad \text{and} \quad \frac{\partial \Omega}{\partial Y_{ij}} = 0. \tag{3.46}$$

Substitution of Eq. (3.45) into Eq. (94) along with Eq. (3.41) yields the thermodynamic laws corresponding to the evolution of the total inelastic deformation rate ($\mathbf{d}^I$) and the viscodamage variable ($\boldsymbol{\phi}$), where Eq. $(4.46)_1$ gives the inelastic deformation rate tensor as follows:

$$d^I_{ij} = \dot{\Lambda}^{vp} \frac{\partial f}{\partial \tau_{ij}} + \dot{\Lambda}^{d} \frac{\partial g}{\partial \tau_{ij}} \tag{3.47}$$

Considering the earlier postulate of the additive decomposition of the inelastic deformation rate into viscoplastic and viscodamage parts (Eq. (2.27)), the following assumption is made:

$$d^{vp}_{ij} = \dot{\Lambda}^{vp} \frac{\partial f}{\partial \tau_{ij}} \quad \text{and} \quad d^{id}_{ij} = \dot{\Lambda}^{d} \frac{\partial g}{\partial \tau_{ij}} \tag{3.48}$$

while Eq. $(4.46)_2$ gives the viscodamage rate evolution law as follows:

$$L_v(\phi_{ij}) = \dot{\Lambda}^{vp} \frac{\partial f}{\partial Y_{ij}} + \dot{\Lambda}^{d} \frac{\partial g}{\partial Y_{ij}} \tag{3.49}$$

where f and g are respectively the dynamic viscoplastic and viscodamage loading surfaces outlined in the following section. Eqs. (3.47) and (3.49) show that a strong coupling exists between viscoplasticity and viscodamage in such a way that $\mathbf{d}^I$ is decomposed into viscoplastic ($\mathbf{d}^{vp}$) and viscoinelastic-damage ($\mathbf{d}^{id}$) components and both $\mathbf{d}^I$ and $\boldsymbol{\phi}$ are expressed in terms of the viscoplastic and viscodamage potentials.

Now, in order to obtain non-associative rules for the viscoplasticity and viscodamage hardening variables, one can assume the existence of a viscoplastic potential F and a viscodamage potential G such that they are respectively not

equal to f and g. This postulate is essential in order to obtain nonlinear viscoplastic and viscodamage hardening rules, which give a more realistic characterzation of the material response in the deformation process. The complementary laws for the evolution of the other internal state variables can then be obtained drectly from the generalized normality rule, which are summarized in Table 3. Those evolution laws show strong viscoplasticity and viscodamage coupling. This strong coupling results, on the one hand, from the fact that the viscoplasticity evolution equations are obtained in the current, deformed, and damaged state and, on the other hand, the damage evolution equations are expressed in terms of the viscoplastic and viscodamage potentials.

It is noteworthy to mention that the Lagrangian parameters $\dot{\Lambda}^{up}$ and $\dot{\Lambda}^{d}$, respectively, characterize the effective or equivalent viscoplastic and viscodamage deformations. Therefore, the evolution of the assumed gradient variables is associated with the gradients of $\dot{\Lambda}^{up}$ and $\dot{\Lambda}^{d}$. This is clearly shown by the evolution equations of $\nabla^2 p, L_v\alpha, \nabla^2 r$, and $L_v\Gamma$ in Table 3.

Table 3. The thermodynamic laws for the evolution of the internal state variables.

Plasticity	Isotropic Hardening Evolution Laws	$\dot{p} = -\dot{\Lambda}^{vp}\frac{\partial F}{\partial R}$, $\overline{\nabla^2 p} = -\nabla^2 \dot{\Lambda}^{vp}\frac{\partial F}{\partial R^g}$
	Kinematic Hardening Evolution Laws	$L_v(\alpha_{ij}) = -\dot{\Lambda}^{vp}\frac{\partial F}{\partial X_{ij}}$, $L_v(\nabla^2\alpha_{ij}) = -\nabla^2\dot{\Lambda}^{vp}\frac{\partial F}{\partial X^g_{ij}}$
Damage	Isotropic Hardening Evolution Laws	$\dot{r} = -\dot{\Lambda}^{d}\frac{\partial G}{\partial K}$, $\overline{\nabla^2 r} = -\nabla^2\dot{\Lambda}^{d}\frac{\partial G}{\partial K^g}$
	Kinematic Hardening Evolution Laws	$L_v(\Gamma_{ij}) = -\dot{\Lambda}^{d}\frac{\partial G}{\partial H_{ij}}$, $L_v(\nabla^2\Gamma_{ij}) = -\nabla^2\dot{\Lambda}^{d}\frac{\partial G}{\partial H^g_{ij}}$

The non-local evolution of each of the assumed internal state variables $L_v\widehat{\Xi}_n$, $(n = 1-4))$ at position x in the current configuration, can be expressed as the weighted average of its local counterpart $L_v\Xi_n$ over a surrounding volune v at a small distance $|\zeta| \leq L_C$ from the considered point, such that:

$$L_v\widehat{\Xi}_n = \frac{1}{v}\int_v h(\zeta)\, L_v\Xi_n(x+\zeta)\, dv, \tag{3.50}$$

where L_c is an internal characteristic length and $h(\zeta)$ is a weight function that decays smoothly with distance and in this work is given by $h(\zeta) = \mathbf{I}h(\zeta)$ where $\mathbf{I}$ is an identity tensor. However, the identity tensor $\mathbf{I}$ may be suitably subsituted

by another tensor in order to induce further anisotropic behavior of the material (VOYIADJIS and DORGAN [97]).The local variable $L_v\Xi_n$ in Eq. (3.50) can be approximated by a Taylor expansion at $\zeta = 0$ such that:

$$L_v\Xi_n(x+\zeta) = L_v\Xi_n(x) + \nabla L_v\Xi_n(x)\,\zeta + \frac{1}{2!}\nabla^2 L_v\Xi_n(x)\,\zeta\zeta + \frac{1}{3!}\nabla^3 L_v\Xi_n(x)\,\zeta\zeta\zeta + \cdots \tag{3.51}$$

where ∇^i denotes the i-th order gradient operator. Assuming only an isotropic influence of the averaging equation, as we stated previously, the integrals of the odd terms in Eq. (3.51) vanish. Furthermore, making use of Eqs. (3.50) and (3.51) and truncating the Taylor series after the quadratic term lead to the following expression for the nonlocal variable $L_v\widehat{\Xi}_n$:

$$L_v\widehat{\Xi}_n = \frac{1}{v}\int_v h(\zeta)\,L_v\Xi_n(x)\,dv + \frac{1}{2v}\int_v h(\zeta)\,\nabla^2 L_v\Xi_n(x)\,\zeta\zeta\,dv. \tag{3.52}$$

This relation can be expressed as a partial differential equation such that:

$$L_v\widehat{\Xi}_n = L_v\Xi_n + \left(\frac{1}{2v}\int_v [h(\zeta)]\,\zeta\zeta\,dv\right)\nabla^2 L_v\Xi_n. \tag{3.53}$$

However, setting $\dfrac{1}{v}\displaystyle\int_v [h(z)]\,dv = 1$, Eq. (3.53) can be re-written at constant x as follows:

$$L_v\widehat{\Xi}_n = L_v\Xi_n + c_n L_v\nabla^2\Xi_n. \tag{3.54}$$

such that:

$$\dot{\widehat{p}} = \dot{p} + c_1\,\dot{\overline{\nabla^2 p}}, \tag{3.55}$$

$$L_v(\widehat{\alpha}_{ij}) = L_v(\alpha_{ij}) + c_2 L_v(\nabla^2\alpha_{ij}), \tag{3.56}$$

$$\dot{\widehat{r}} = \dot{r} + c_3\,\dot{\overline{\nabla^2 r}}, \tag{3.57}$$

$$L_v(\widehat{\Gamma}_{ij}) = L_v(\Gamma_{ij}) + c_4 L_v(\nabla^2\Gamma_{ij}). \tag{3.58}$$

In Eqs. (3.54)-(3.59), $(n = 1-4)$ are constants proportional to length squared and weight each component of the gradient term identically, which give a rise for explicit length-scale measures. If one assumes a more general tensorial character for $\mathbf{h}$ not necessarily confined to the expression in terms of an identity tensor, then one obtains a different weighting of the individual coefficients. This will give a weighting function with a tensorial nature c_n containing several different integration constants.

Following Eq. (3.54), one can write the evolution equations of the corresponding non-local state laws as follows:

$$L_v\widehat{\Sigma}_n = L_v\Sigma_n + L_v\Sigma_n^g \tag{3.59}$$

such that:

$$\dot{\widehat{R}} = \dot{R} + \dot{R}^g, \tag{3.60}$$

$$L_v(\widehat{X}_{ij}) = L_v(X_{ij}) + L_v(X_{ij}^g), \tag{3.61}$$

$$\dot{\widehat{K}} = \dot{K} + \dot{K}^g, \tag{3.62}$$

$$L_v(\widehat{H}_{ij}) = L_v(H_{ij}) + L_v(H_{ij}^g). \tag{3.63}$$

The next important step is the selection of the appropriate form of the viscoplastic potential function $F \geq 0$ and the viscodamage potential function $G \geq 0$ in order to establish the desired constitutive equations that describe the mechanical behavior of the material. It is clearly seen in the previous part of this work that the viscodamage evolution laws are strongly coupled with viscoplasticity. To maintain this strong coupling, two independent viscodamage mechanisms are distinguished. One mechanism is coupled with viscoplasticity, while the other one occurs independent of viscoplastic deformation. Similar argument was presented by HESEBECK [46], where he showed that the first mechanism is dominated in the case of shear stress and the second one for hydrostatic stress. In order to be consistent and satisfy the generalized normality rule of thermodynamics, a proper analytical form for the viscoplastic and the viscodamage potentials need to be postulated to obtain consistent evolution equations for the flux variables, such that:

$$F = f + \frac{1}{2}k_1\bar{X}_{mn}\bar{X}_{mn} + \frac{1}{2}k_2\bar{X}_{mn}^g\bar{X}_{mn}^g + \frac{1}{2}k_3\bar{R}^2 + \frac{1}{2}k_4\bar{R}^{g^2}, \tag{3.64}$$

$$G = g + \frac{1}{2}k_5 \mathrm{H}_{mn}\mathrm{H}_{mn} + \frac{1}{2}k_6 \mathrm{H}^g_{mn}\mathrm{H}^g_{mn} + \frac{1}{2}k_7 K^2 + \frac{1}{2}k_8 K^{g^2}, \tag{3.65}$$

where k_i $(i = 1 - 8)$ are material constants used to adjust the units of the equation, which are again independent of temperature. $\bar{X}$ and $\bar{X}^g$ are the effective backstress tensors associated with the kinematic hardening and are expressed similarly to Eq. (2.29) as:

$$\bar{X}_{ij} = M_{ikjl}X_{kl} \quad \text{and} \quad \bar{X}^g_{ij} = M_{ikjl}X^g_{kl}. \tag{3.66}$$

The isotropic hardening represents a global expansion in the size of the yield surface with no change in shape. Thus for a given yield criterion and flow rule, isotropic hardening in any process can be predicted from the knowledge of the functions $\bar{R}$ and $\bar{R}^g$, and those functions may in principle, be determined from a single test (e.g. the tension test). Therefore, the effective isotropic hardening functions $\bar{R}$ and $\bar{R}^g$ are related to the nominal isotropic hardening function R and R^g similar to Eq. (2.29) as follows:

$$\bar{R} = \frac{R}{1-r}, \tag{3.67}$$

$$\bar{R}^g = \frac{R^g}{1-r}, \tag{3.68}$$

where r is defined as the accumulative or equivalent damage and can be expressed as follows:

$$r = \sqrt{\phi_{ij}\phi_{ij}}\,. \tag{3.69}$$

The assumed potential functions indicate the need for two loading surfaces f and g, one for viscoplasticity and another for viscodamage, respectively. Thus, the coupled anisotropic viscoplastic and viscodamage formulation is a two-surface model whereby anisotropic viscodamage is formulated in the spirit of viscoplasticity, complete with a viscodamage criterion and flow rules.

4. Viscoplasticity yield criterion and its corresponding flow rules

4.1. Viscoplasticity yield criterion

Once a material is damaged, further loading can only affect the undamaged material. Thus, the viscoplastic function f is defined in terms of the effective stresses. For the classical J_2 rate-independent plasticity, the static yield surface f_s (at negligible viscoplastic strain rate) is assumed to be of a von Mises type with isotropic and kinematic hardening, and defined as follows:

$$f_s = \sqrt{3J_2\left(\bar{\tau}'_{ij} - \bar{X}_{ij} - \bar{X}^g_{ij}\right)} - \bar{\tau}_{yp}(T) - \bar{R}\left(\bar{p}, T\right) - \bar{R}^g\left(\nabla^2\bar{p}, T\right) \leq 0 \tag{4.1}$$

where $J_2 = 1/2(\bar{\tau}' - \bar{X} - \bar{X}^g) : (\bar{\tau}' - \bar{X} - \bar{X}^g)$ is the second invariant of the deviatoric stress tensor $(\bar{\tau}' - \bar{X} - \bar{X}^g)$, $\bar{\tau}_{yp}(T)$ is the initial yield strength as a function of temperature, R and R^g are the isotropic hardening functions, T is the absolute temperature, and $\bar{p}$ is the equivalent viscoplastic strain. $\bar{\boldsymbol{\tau}}'$ is the effective deviatoric Kirchhoff stress tensor, $\bar{X}$ and $\bar{X}^g$ are the effective backstress tensors associated with the kinematic hardening. $\bar{\boldsymbol{\tau}}'$ is expressed in terms of the viscodamage tensor M (given by Eq. (2.30)) and the corresponding damage states as follows (VOYIADJIS and KATTAN [100]):

$$\bar{\tau}'_{ij} = M'_{ijkl}\tau_{kl} \quad \text{with} \quad M'_{ijkl} = M_{ijkl} - \frac{1}{3}M_{rrkl}\delta_{ij}. \tag{4.2}$$

The accumulative or equivalent rate of the effective viscoplastic deformation $(\dot{\bar{p}})$ is defined by:

$$\dot{\bar{p}} = \sqrt{\frac{2}{3}\bar{d}^{vp}_{ij}\bar{d}^{vp}_{ij}} \tag{4.3}$$

where $\bar{\mathbf{d}}^{vp}$ is the viscoplastic deformation rate tensor in the effective configuration.

The extension of Eq. (4.1) to include the rate-dependent plasticity (viscoplasticity) implies that the stress state is no longer constrained to remain on the yield surface but one can have$f_s \geq 0$. Therefore, we define the dynamic yield surface f as follows:

$$f = \sqrt{3J_2\left(\bar{\tau}'_{ij} - \bar{X}_{ij} - \bar{X}^g_{ij}\right)} - \bar{\tau}_{yp} - \bar{R} - \bar{R}^g - \bar{\tau}_{vp} \equiv 0 \tag{4.4}$$

where $\bar{\tau}_{vp} = \langle f_s \rangle$ is the viscous effective stress (or the overstress, i.e. the difference between the dynamic stress and its static counterpart) and $\langle x \rangle$ denotes the MacAuley brackets defined by $\langle x \rangle = (x + |x|)/2$. Clearly, $\bar{\tau}_{vp}$ is the common notion of viscoplasticity (PERZYNA [78]), which implies that an inelastic process can only take place if, and only if, the overstress $\bar{\tau}_{vp}$ is positive. From the assumed yield function f the current effective yield stress can be defined as follows to account for high-strain rate and temperature effects:

$$\bar{Y} = \bar{\tau}_{yp}(T) + \bar{R}(\bar{p}, T) + \bar{R}^g\left(\nabla^2\bar{p}, T\right) + \bar{\tau}_{vp}\left(\dot{\bar{p}}, \nabla^2\dot{\bar{p}}, \bar{p}, \nabla^2\bar{p}, T\right) \tag{4.5}$$

where one can define the initial yield strength $\bar{\tau}_{yp}$ as follows:

$$\bar{\tau}_{yp}(T) = \bar{\sigma}_o\vartheta \tag{4.6}$$

where $\bar{Y}_o$ is the initial yield stress in the undamaged state, which is obtained at zero absolute temperature, zero viscoplastic strain, and static strain rate, and

$\vartheta = 1-(T/T_m)^n$. The evolution equations of the hardening functions $\bar{R}$, $\bar{R}^g$, $\bar{X}$, and $\bar{X}^g$ will be derived in the subsequent sections.

The proposed dynamic yield criterion $f = 0$ (Eq. (4.4)) is a generalization of the classical von Mises yield criterion $f_s \leq 0$ (Eq. (4.1)) for rate-dependent materials. The latter can be simply recovered by imposing $\dot{p} = \dot{p}_o$ (rate-independent), so that one has the plasticity case $f \leq 0$, where $\dot{p}_0$ is the static strain rate (i.e. the smallest strain rate of the strain-rate range considered), and is called the control strain rate according to the notation of PERZYNA [81]. In the elastic domain, both f_s and f are equivalent since, in that case, $\dot{p} = 0$. Therefore, the admissible stress states are constrained to remain on or within the elastic domain ($f \leq 0$). The viscoplastic parameter $\dot{\Lambda}^{vp} \geq 0$, which is known as the plastic consistency parameter, is assumed to obey the following Kuhn-Tucker loading/unloading conditions (SIMO and HUGHES, 1998):

$$f \leq 0 \quad \text{and} \quad \dot{f} \left\{ \begin{array}{ll} < 0 & \Rightarrow \dot{\Lambda}^{vp} = 0 \\ = 0 & \Rightarrow \dot{\Lambda}^{vp} = 0 \\ = 0 & \Rightarrow \dot{\Lambda}^{vp} > 0 \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} \text{elastic unloading} \\ \text{neutral loading} \\ \text{plastic loading} \end{array} \right. \tag{4.7}$$

Thus, f still satisfies the constraint equation Eq. (3.45) and the maximum dissipation principle Eq. $(94)_1$.

4.2. Viscoplastic flow rule d^{vp}

One can substitute in Eq. $(4.48)_1$ different admissible forms for the Lagrange multiplier $\dot{\Lambda}^{vp}$ without violating the constrained maximization problem presented by Eq. $(4.46)_1$. However, the evolution equation for $\dot{\Lambda}^{vp}$ is now defined in a quiet similar way as in the classical viscoplasticity. Several evolution equations have been proposed in the literature to calculate the viscoplastic strain rate. Some of them are physically-based and others are phenomenological. The most widely used in rate-dependent plasticity (viscoplasticity) are those based on the overstress concept (ZENER and HOLLOMON [108], [109], MALVERN [65], [66], PERZYNA [77], [78], [80], [83]). One of the first and most widely used phenomenological models for rate-sensitive plastic flow is due to PERZYNA ([77], [78], [79], [80], [81]), which has been often considered in computational applications. On the other hand, ZENER and HOLLOMON ([108], [109]) proposed that the functional dependence of the magnitude of the inelastic strain rate of metals could be multiplicatively decomposed into two functions: thermal (static) and stress (dynamic). FREED and WALKER ([37], [39]) and FREED *et al.* [38] showed that the Zener parameter is very general and includes many viscoplastic theories as special cases. In the spirit of the Perzyna-type and Zener-type evolution equations for the viscoplastic strain rate, one can postulate the following admissible

form for the Lagrangian multiplier $\dot{\Lambda}^{vp}$, such that:

$$\dot{\Lambda}^{vp} = \frac{1}{\eta_{vp}} \left[\frac{\langle \bar{\tau}_{vp} \rangle}{\bar{\tau}_{yp} + \bar{R} + \bar{R}^g} \right]^{m_1} \tag{4.8}$$

where m_1 is the viscoplastic rate sensitivity parameter and η_v is the viscosity or fluidity parameter, sometimes referred to as the relaxation time according to notation of PERZYNA [81]. Note that the script "vp" used as a superscript or subscript does not designate tensor indices but hardly denotes the corresponding viscoplasticity.

One can now utilize the hypothesis of viscoplastic dissipation equivalence Lee *et al.* [58], VOYIADJIS and THIAGARAJAN [103], VOYIADJIS and DELIKTAS [95]. This hypothesis assumes that the viscoplastic energy in terms of the effective and nominal stress and strain quantities must be equal. Thus, one can write the following relation, such that:

$$\bar{d}_{ij}^{vp} = N_{ikjl} d_{kl}^{vp} \tag{4.9}$$

where N is the inverse of the fourth-order damage tensor which is given by Eq. (2.32).

By making use of the effective stress equation (Eq. (2.29)) and the effective viscoplastic deformation rate equation (Eq. (4.9)), we can write the viscoplastic deformation rate equation (Eq. $(96)_1$) as follows:

$$\bar{d}_{ij}^{vp} = \dot{\Lambda}^{vp} \frac{\partial f}{\partial \bar{\tau}_{ij}}, \tag{4.10}$$

Since $\partial f / \partial \bar{\tau} : \partial f / \partial \bar{\tau} = 1.5$, it can be easily shown that the effective rate of the accumulative viscoplastic deformation rate ($\dot{\bar{p}}$) defined by Eq. (4.3) is related to $\dot{\nabla}^{vp}$ by:

$$\dot{\bar{p}} = \dot{\Lambda}^{vp}, \tag{4.11}$$

By making use of Eqs. (4.8) and (4.11), one can write an expression for the overstress function $\bar{\tau}_{vp}$ as follows:

$$\bar{\tau}_{vp} = \left(\eta_{vp} \dot{\bar{p}}\right)^{1/m_1} \left(\bar{\tau}_{yp} + \bar{R} + \bar{R}^g\right). \tag{4.12}$$

Note that from Eq. (4.12) the classical von Mises criterion $f_s = 0$ (Eq. (4.1)) for rate-independent materials can be simply recovered by imposing $\eta_{vp} = 0$ (no viscosity effect) on f (Eq. (4.4)). Moreover, the well-known fact that, from the relation in Eq. (4.8), it can be noted that as the viscosity parameter η_{vp} goes to zero, the consistency parameter $\dot{\nabla}^{vp}$ remains finite and positive (though indeterminate) since $\bar{\tau}_v$ also goes to zero.

Setting the dynamic yield function f in the proposed form allows one to use effectively the well-known rate-independent radial-return algorithm to integrate the viscoplasticity governing equations. Applying the consistency condition, $\dot{f} = 0$, also gives $\dot{\Lambda}^{vp}$ as proposed in Eq. (4.8).

4.3. Viscoplastic hardening rules

Now, in order to derive the evolution of the viscoplasticity isotropic hardening functions $\bar{R}$ and $\bar{R}^g$ in the effective state to be used in the dynamic yield function f, we makes use of Eqs. (3.64), (3.67), (3.68), (4.4), and (4.11) in $\dot{p}$ and $\overline{\nabla^2 p}$ equations in Table 3 along with the chain rule, such that the following expressions can be written :

$$\dot{p} = \frac{\dot{\bar{p}}}{1-r}\left(1 - k_3\bar{R}\right), \tag{4.13}$$

$$\overline{\nabla^2 p} = \frac{\nabla^2\dot{\bar{p}}}{1-r}\left(1 - k_4\bar{R}^g\right). \tag{4.14}$$

By operating on R and R^g relations in Table 2, and $\bar{R}$ and $\bar{R}^g$ relations (Eqs. (3.67) and (3.68)) with the Lie derivative for a given temperature and keeping the damage history constant (i.e. the damage internal state tensor $\boldsymbol{\Phi}$ and temperature T are kept constant), one can write the following evolution equations for $\bar{R}$ and $\bar{R}^g$, respectively, as follows:

$$\dot{\bar{R}} = \frac{a_1\dot{\bar{p}}}{(1-r)^2}\left(1 - k_3\bar{R}\right)\vartheta \tag{4.15}$$

$$\dot{\bar{R}}^g = \frac{a_2\nabla^2\dot{\bar{p}}}{(1-r)^2}\left(1 - k_4\bar{R}^g\right)\vartheta \tag{4.16}$$

Now in order to derive the kinematic hardening evolution equations associated with viscoplasticity, one makes use of $L_v\alpha$ equation in Table 3 along with the chain rule and Eq. $(114)_1$, such that one can write the following:

$$L_v(\alpha_{ij}) = -\dot{\Lambda}^{vp} M_{minj}\frac{\partial F}{\partial \bar{X}_{mn}}, \tag{4.17}$$

Substitution of Eq. (3.64) into the above equation yields:

$$L_v(\alpha_{ij}) = -\dot{\Lambda}^{vp} M_{minj}\left(\frac{\partial f}{\partial \bar{X}_{mn}} + k_1\bar{X}_{mn}\right), \tag{4.18}$$

Since $\partial f/\partial \bar{X} = -\partial f/\partial \bar{\tau}$ as it is clear from Eq. (4.1), it can be easily shown by using Eqs. (4.10) and (4.11) that Eq. (4.18) can be rewritten as follows:

$$L_v(\alpha_{ij}) = M_{minj}\left(\bar{d}^{vp}_{mn} - k_1\dot{\bar{p}}\bar{X}_{mn}\right). \tag{4.19}$$

However, operating on the X relation in Table 2, and $\bar{X}$ relation Eq. $(114)_1$ with the Lie derivative for a given temperature and keeping the damage history constant (i.e. the viscodamage effective tensor $\mathbf{M}$ and temperature T are kept constant), one can write the following evolution equation for $\bar{X}$ as follows:

$$L_v(\bar{X}_{ij}) = \mathbf{M}_{ikjl}\mathbf{M}_{mknl}\left(a_3\bar{d}^{vp}_{mn} - k_1 a_3\dot{\bar{p}}\bar{X}_{mn}\right)\vartheta. \tag{4.20}$$

When the infinitesimal deformations and rate and temperature-independent response of a material are assumed and the micro-damage effects are neglected then the kinematic hardening law (Eq. (4.20)) reduces to that proposed by ARMSTRONG and FREDERICK [6].

Similarly, by utilizing $L_v\nabla^2\alpha$ equation in Table 3 and the Lie derivative of X^g relation in Table 2, one can write the gradient-dependent evolution equation of viscoplasticity kinematic hardening $(L_v X^g)$ as:

$$L_v(\bar{X}^g_{ij}) = M_{ikjl}M_{mknl}\left(a_4\frac{\partial f}{\partial \bar{\tau}_{mn}} - k_2 a_4 \bar{X}^g_{mn}\right)\nabla^2\dot{\bar{p}}\vartheta \tag{4.21}$$

It is noteworthy to point out here that the derived evolution equations of viscoplasticity hardening ($\dot{\bar{R}}$, $\dot{\bar{R}}^g$, $L_v X$, and $L_v X^g$) containing hardening terms that represent the strengthening mechanism as well as recovery terms that represent the softening mechanism. Both the hardening and recovery terms are affected by the static (thermal) recovery term ϑ in such a way that the functional dependence of the hardening of materials could be multiplicatively decomposed into two functions: thermal (static) and stress (dynamic). Therefore, those evolution equations characterize the time and thermal effects due to the rate and temperature dependence. FREED *et. al.* [38] pointed out that in viscoplasticity at elevated temperatures, thermal recovery of materials usually plays an important rule in the deformation process. In impact-related problems, the thermomechanical response of the assumed internal state variables is strongly dependent on the temperature history. This requires existence of thermal recovery (softening) terms in the evolution equations of the internal state variables.

4.4. Damage evolution criterion and its corresponding flow rules

4.4.1. Damage evolution criterion. By combining viscoplasticity with viscodamage, it seems natural that damage can only affect the undamaged material skeleton. Thus the viscodamage function g is also defined in terms of the effective

stresses. The anisotropic viscodamage calculation is formulated in spirit of viscoplasticity; therefore, analogous to the dynamic viscoplastic yield surface presented in the previous section, the dynamic viscodamage surface g which evolves from a static damage surface g_s can be postulated as follows:

$$g = g_s - L(T, r, \dot{r}, \overline{\nabla^2 r}) = 0 \tag{4.22}$$

$$g = \sqrt{J_2(Y_{ij} - H_{ij} - H^g_{ij})} - l\,(T) - K\,(r,T) - K^g\left(\nabla^2 r, T\right) - L(T, r, \nabla^2 r, \dot{r}, \overline{\nabla^2 r}) = 0 \tag{4.23}$$

where $J_2(Y - H - H^g)$ denotes the second invariant of the damage force $(Y - H - H^g)$, $l(T)$ is the initial damage threshold as a function of temperature, and L is the threshold damage force increment for microdamge nucleation, growth, and coalescence, which is dependent on the temperature, damage accumulation, and rate of damage accumulation.

Similar expressions for $l(T)$ and $\dot{\Lambda}^d$ can be postulated as presented by Eqs. (4.6) and (4.8), respectively, such that:

$$l\,(T) = l_o \vartheta, \tag{4.24}$$

$$\dot{\Lambda}^d = \frac{1}{\eta_{vd}} \left[\frac{\langle L \rangle}{l + K + K^g}\right]^{m_2}, \tag{4.25}$$

where l_o is the initial damage threshold at zero absolute temperature, zero damage strain, and static damage strain rate, and $\vartheta = 1 - (T/T_m)^n$. m_2 is the damage rate sensitivity parameter and η_{vd} is the viscosity parameter or the damage relaxation time, which can be different than η_{vp}.

By making use of Eq. (4.25), one can write an expression for the overforce damage function L as follows:

$$L = (\eta_{vd}\dot{r})^{1/m_2}\,(l + K + K^g)\,. \tag{4.26}$$

The postulated dynamic viscodamage function $g = 0$ (Eq. (4.23)) is a generalization of the static damage surface as proposed by Voyiadjis and Deliktas (2000b) for rate-dependent materials. Similar to the yield surface, the static damage surface can be simply recovered by imposing $\eta_{vd} = 0$ (rate-independent), so that one has the instantaneous damage case $g \leq 0$. In the undamaged domain, both the static and dynamic damage growth conditions are equivalent since, in that case, $\dot{r} = 0$. Therefore, the admissible damage forces are constrained to

remain on or within the undamaged domain ($g \leq 0$). The model response in the viscodamage domain is then characterized as follows:

$$g = g_s < 0 \Leftrightarrow \text{undamaged state} \Rightarrow \dot{\nabla}^d = 0, \tag{4.27}$$

$$g \leq 0 \quad \text{and} \quad \dot{g} \begin{cases} < 0 \Rightarrow \dot{\Lambda}^d = 0 \\ = 0 \Rightarrow \dot{\Lambda}^d = 0 \\ > 0 \Rightarrow \dot{\Lambda}^d > 0 \end{cases} \Leftrightarrow \begin{cases} \text{undamaged state} \\ \text{damage initiation} \\ \text{damage growth} \end{cases} \tag{4.28}$$

4.4.2. Damage hardening rules. Now, in order to derive the hardening evolution equations associated with viscodamage process, we follow the same procedure presented in the previous section for viscoplasticity. The evolution equations for the viscodamage isotropic hardening functions K and K^g are obtained by making use of Eqs. (3.65) and (4.23) in $\dot{r}$ and $\overline{\nabla^2 r}$ relations in Table 3 along with the Lie derivative of K and K^g equations in Table 2 for a given temperature, such that the following expressions are obtained:

$$\dot{K} = b_1 (1 - k_7 K) \dot{r}\vartheta \tag{4.29}$$

$$\dot{K}^g = b_2 (1 - k_8 K^g) \nabla^2 \dot{r}\vartheta \tag{4.30}$$

Moreover, the viscodamage kinematic hardening evolutions equations can be obtained by using $L_v\Gamma$ and $L_v\nabla^2\Gamma$ relations in Table 3 and Eq. (3.65), such that one obtains the following:

$$L_v(\Gamma_{ij}) = -\dot{\Lambda}^d \left(\frac{\partial g}{\partial H_{ij}} + k_5 H_{ij} \right), \tag{4.31}$$

$$L_v(\nabla^2 \Gamma_{ij}) = -\nabla^2 \dot{\Lambda}^d \left(\frac{\partial g}{\partial H^g_{ij}} + k_6 H^g_{ij} \right), \tag{4.32}$$

Since $\partial g/\partial H = \partial g/\partial H^g = -\partial g/\partial Y$ as it is clear from Eq. (4.23) it can be easily shown by taking the Lie derivative of H and H^g equations in Table 2 for a given temperature that Eqs. (4.31) and (4.32) can be rewritten as follows:

$$L_v(H_{ij}) = \left(b_3 \frac{\partial g}{\partial Y_{ij}} - k_5 b_3 H_{ij} \right) \dot{r}\vartheta \tag{4.33}$$

$$L_v(H^g_{ij}) = \left(b_4 \frac{\partial g}{\partial Y_{ij}} - k_6 b_4 H^g_{ij} \right) \nabla^2 \dot{r}\vartheta. \tag{4.34}$$

Similar to the viscoplastic hardening evolution equations, the derived viscodamage evolution equations consider the dynamic recovery as well as the static recovery (thermal recovery). Besides, the static recovery occurs in both the hardening and the dynamic recovery terms. The hardening term of each assumed internal state variable accounts for strengthening mechanisms, while the recovery terms account for softening mechanisms.

For the sake of completeness, we outline in the Appendix the derivatives that are necessary to calculate the above derived evolution equations.

5. Rate-type constitutive relation

As previously mentioned, the elasticity tensor $\Im$ can be considered constant either in the material or current configuration. This leads to the definition of different materials. We are going to consider here that the elasticity tensor $\Im$ is constant in the reference configuration C^o. Therefore, operating on the stress relation Eq. (3.30) with the Lie derivative and keeping the damage history constant (i.e. the internal state variables ϕ constant), one can obtain for a general thermo-elasto-viscoplastic and viscodamage flow processes the following relation:

$$L_v(\tau_{ij}) = \Im_{ijkl}\left(d_{kl} - d^{vp}_{kl} - d^{id}_{kl}\right) - \beta_{ij}\dot{T} \tag{5.1}$$

where $\Im$ is the spatial elasticity-damage tensor related to the fourth-order tensor of elastic-damaged constants C (Eq. (2.31)) by the (push-forward) transformation as follows:

$$\Im_{ijkl} = F_{ir}F_{js}F_{km}F_{ln}C_{rsmn}. \tag{5.2}$$

Similarly, Eqs. (5.1) and (5.2) can be defined, respectively, using the Jaumann-Zaremba stress rate tensor as follows:

$$\tau^o_{ij} = a_{ijkl}\left(d_{kl} - d^{vp}_{kl} - d^{id}_{kl}\right) - \beta_{ij}\dot{T} \tag{5.3}$$

where

$$a_{ijkl} = \Im_{ijkl} + \delta_{il}\tau_{jk} + \delta_{jl}\tau_{ik}. \tag{5.4}$$

Substitution of Eqs. (4.48), (4.8) and (4.25) into Eq. (5.3), yields:

$$\tau^o_{ij} = a_{ijkl} \cdot \left[d_{kl} - \frac{1}{\eta_v}\left\langle\frac{\bar{\tau}_v}{\bar{\tau}_{yp} + \bar{R} + \bar{R}^g}\right\rangle^{m_1}\frac{\partial f}{\partial \tau_{kl}} - \frac{1}{\eta_{vd}}\left\langle\frac{L}{l + K + K^g}\right\rangle^{m_2}\frac{\partial g}{\partial \tau_{kl}}\right] - \beta_{ij}\dot{T}. \tag{5.5}$$

6. Thermomechanical couplings

Substituting Ψ from Eq. (3.14) into Eq. (3.11) yields the following energy balance equation:

$$\rho\left(\dot{\Psi}+\eta\dot{T}+\dot{\eta}T\right)-\frac{\rho}{\rho^o}\tau_{ij}d_{ij}-\rho h+q_{i,i}=0 \tag{6.1}$$

Substituting $\dot{\Psi}$ (Eq. (3.17)) into the above equality and taking into account the results presented by Eqs. (3.23) and (3.40) we obtain the following:

$$\rho^o\dot{\eta}T=\tau_{ij}\left(d_{ij}^{vp}+d_{ij}^{id}\right)-\Pi_{int}+\rho^o h+Jq_{i,i}=0 \tag{6.2}$$

Operating on the entropy relation Eq. $(3.23)_2$ with the Lie derivative and substituting the result into Eq. (6.2), we obtain:

$$\rho c_p\dot{T}=\Upsilon\frac{\rho}{\rho^o}\tau_{ij}^{'}\left(d_{ij}^{vp}+d_{ij}^{id}\right)+\Upsilon\frac{\rho}{\rho^o}P\left(d_{ij}^{vp}+d_{ij}^{id}\right)-\rho\Pi_{int}+\rho\frac{\partial\Sigma_k}{\partial T}\dot{\aleph}_kT - \frac{\rho}{\rho^o}\beta_{ij}d_{ij}^{E}T+\rho^o r_{ext}+k\nabla^2T \tag{6.3}$$

where $c_p=T\partial\eta/\partial T$ is the specific heat at constant pressure.

The rate type-equations (Eqs. (5.5) and (6.3)) take into account effects of the viscoplastic and viscodamage strain-induced anisotropy (i.e. kinematic hardening), flow stress temperature and strain-rate sensitivity (i.e. isotropic hardening), anisotropic damage (i.e. softening generated by damage defects nucleation and growth mechanisms), thermomechanical couplings (i.e. thermal viscoplastic and viscodamage softening), strong viscoplasticity and viscodamage coupling, and heterogeneity in the material behavior (i.e. the non-local influence).

7. Conclusions

A thermodynamically consistent nonlocal gradient-enhanced framework is presented here with strong viscoplasticity and anisotropic viscodamage coupling for impact-related problems. Thermodynamically consistent constitutive equations are derived in order to introduce issues such as the statistical inhomogeneity in the evolution-related viscoplasticity and viscodamage variables associated with the RVE, localization and size effects of deformation defects on the macroscopic response of heterogeneous materials, and temperature and strain-rate sensitivity.

This model is general enough to describe the evolution of visco-inelasticity in a material body accounting for physical discontinuities through the use of

a nonlocal approach based on the gradient-dependent theory of viscoplasticity and viscodamage. The interaction of the length-scales is a crucial factor in understanding and controlling the material defects such as mobile and immobile dislocation densities, voids, and cracks influence on the macroscopic response. The behavior of these defects is captured not only individually, but also the enhanced strong coupling between the two dissipative processes takes into account the interaction between these defects and their ability to create spatio-temporal patterns under different loading conditions. An equation of state is presented in this work for high impact loading that accounts for compressibility effects (change in density) in terms of the nominal volumetric damage strain.

Length-scale parameters are implicitly and explicitly introduced into the present dynamical formulation. Implicit length-scale measure is introduced through the use of the rate-dependent theory, while explicit length-scale measures are introduced through the use of the gradient-dependent theory.

The computational issue of this theoretical formulation with proper explanation of the proper boundary conditions associated with the gradients and evaluation of respective material parameters will be presented in a forthcoming work. Calibration for the different material properties in the proposed approach may be difficult, or impossible for certain cases. However, the proposed framework is generalized to that of viscoplasticity coupled with viscodamage, and one needs more studies to be performed in order to effectively assess the potential applications of this framework.

Appendix

The following relations are necessary for model implementation:

$$Y_{ij} = 2\bar{\Psi}^E M_{kplq} J_{kplqij} \tag{A.1}$$

where $\bar{\Psi}^E$ is given by:

$$\bar{\Psi}^E = \frac{1}{2}\bar{\tau}_{ij}\bar{\Im}^{-1}_{ijkl}\bar{\tau}_{kl} = \frac{1}{2}\tau_{ij}\Im^{-1}_{ijkl}\tau_{kl}, \tag{A.2}$$

and J is a sixth-order tensor and is given by:

$$J_{kplqab} = -\frac{\partial M^{-1}_{kplq}}{\partial \phi_{ab}} = \frac{1}{2}\left(\delta_{lq}\delta_{ka}\delta_{pb} + \delta_{kp}\delta_{la}\delta_{qb}\right), \tag{A.3}$$

$$\frac{\partial f}{\partial \tau_{ij}} = \frac{\partial f}{\partial \bar{\tau}_{mn}}\frac{\partial \bar{\tau}_{mn}}{\partial \tau_{ij}} = M_{minj}\frac{\partial f}{\partial \bar{\tau}_{mn}}, \tag{A.4}$$

$$\frac{\partial g}{\partial \tau_{ij}} \equiv \frac{\partial g}{\partial Y_{mn}} \frac{\partial Y_{mn}}{\partial \tau_{ij}} = e^E_{ij} \frac{\partial g}{\partial Y_{mn}} M_{kplq} J_{kplqmn}, \tag{A.5}$$

$$\frac{\partial f}{\partial Y_{ij}} \equiv \frac{\partial f}{\partial \tau_{mn}} \frac{\partial \tau_{mn}}{\partial Y_{ij}} = \frac{\partial f}{\partial \tau_{mn}} \left(\frac{\partial Y_{ij}}{\partial \tau_{mn}} \right)^{-1}, \tag{A.6}$$

where

$$\frac{\partial Y_{ij}}{\partial \tau_{mn}} = M_{kplq} J_{kplqij} e^E_{mn}, \tag{A.7}$$

$$\frac{\partial g}{\partial Y_{ij}} \equiv \frac{Y_{ij} - H_{ij} - H^g_{ij}}{\sqrt{J_2 \left(Y_{kl} - H_{kl} - H^g_{kl} \right)}}, \tag{A.8}$$

$$\frac{\partial f}{\partial \bar{\tau}_{ij}} \equiv \frac{3}{2} \frac{\bar{\tau}'_{ij} - \bar{X}_{ij} - \bar{X}^g_{ij}}{\sqrt{3 J_2 \left(\bar{\tau}'_{ij} - \bar{X}_{kl} - \bar{X}^g_{ij} \right)}}. \tag{A.9}$$

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On the asymptotic partition of energy in the theory of swelling porous elastic soils

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THE CESÀRO MEANS of various parts of the total energy are introduced in the context of the linear theory of swelling porous elastic soils. Then, the relations describing the asymptotic behavior of the Cesàro means are established.

1. Introduction

IT IS ACCEPTED that the swelling of soils, drying of fibers, wood, plants, paper, etc. are problems concerning the porous media theory. Several recent articles describe the work on the subject and introduce theories for fluids infiltrating elastic media (see [1, 2] and references therein). Most research, in this area, is devoted to some modification of the classical diffusion theory [3]: solids are considered be not to deformable, fluids incompressible and inertial forces are negligible. So, the main physics are diffusion and solid transport. On the other, hand the classical mixture theory approach has been applied to derive a comprehensive macroscopic constitutive theory for swelling porous media (see [4, 5, 6, 7]). A presentation of the continuum theory of mixtures can be found in review articles by BOWEN [8], ATKIN and CRAINE [9, 10] and BEDFORD and DRUMHELLER [11]. In these works, constitutive equations and equations of motion, for mixtures consisting of arbitrary number of fluids and elastic solids, have been obtained.

In [4], ERINGEN has developed a continuum theory for a mixture consisting of three components: an elastic solid, viscous fluid and gas. The intended applications of the theory are in the field of swelling, oil exploration, slurries and consolidation problems. The theory is relevant to problems in the oil exploration industry, since oil is viscous and is usually accompanied by gas in underground rocks, porous solid in slurries and muddy river beds. Consolidation problems in the building industry, earthquake problems, swelling of plants and living tissues and a plethora of other problems fall into the domain of mixture theory considered in [4]. It is also shown that the diffusion-type theories are special cases of the present theory. We note that the theory can be extended in order to incorporate other effects, disregarded here. In this sense, Eringen pointed out: "In some cases, it may be necessary to consider additional properties of mixtures.

For example, elastic solid and/or viscous fluid may require the consideration of memory effects. This is the case for viscoelastic materials..., dislocation problems require consideration of non–local effects. In these problems, stress at a point depends on strains at all points in the body. Plastic deformations of soils and mechanics of sands are problems that require consideration of permanent deformations. These are crucial to the building industry. This divergence is made here to point out to the vast field of mixture theories that are waiting future developments."

In the present paper we continue the study of fundamental qualitative properties of Eringen's mixture theory [4], that began with the papers [12, 13, 14, 15]. Such studies are important to assess whether a given theory is mathematically acceptable for use in a given physical problem. The purpose of this work is to investigate the asymptotic partition of total energy within the context of isothermal linear theory of swelling porous elastic soils.

The question of partition of energy in the asymptotic form was first studied by LAX and PHILLIPS [16] and BRODSKY [17]. Further, this problem has been studied by GOLDSTEIN [18, 19], DUFFIN [20], LEVINE [21]. In his analysis of the abstract wave equation, Goldstein applied the semigroup theory in order to obtain an equipartition theorem stating that the difference of the kinetic energy and the potential energy vanishes as the time approaches infinity. LEVIN [21] treated an abstract version of Goldstein's approach by use of the Lagrange identity method. His result represents a simplified proof that asymptotic equipartition occurs between the Cesàro means of the kinetic and potential energies, a fact first demonstrated by GOLDSTEIN [19].

The asymptotic equipartition between the mean kinetic and strain energies within the context of linear elastodynamics was established by DAY [22]. In the classical linear theory of thermoelasticity, Chiriţă [23] proved that the mean thermal energy tends to zero as time goes to infinity and the asymptotic equipartition occurs between the Cesàro means of the kinetic and strain energies.

This article describes the temporal behavior of solutions to the initial boundary value problems associated with the isothermal linear theory of swelling porous elastic soils. Using the method developed by Chiriţă [23], we introduce the Cesàro means of the kinetic, internal and dissipation energies. Then, with the aid of some auxiliary Lagrange–Brun identities derived in [14], we establish the relations that describe the asymptotic behavior of mean energies. In fact, we prove that asymptotic equipartition occurs between the Cesàro means of the kinetic and internal energies. Therefore, the results established by Day [22] and Chiriţă [23], for elasticity and thermoelasticity, concerning Cesàro means of the energies continue to hold (with corresponding modifications) in the framework of dynamic linear theory of swelling porous elastic soils.

The method developed in [23] has also been used in [24] to study the temporal behavior of solutions in the linear thermoelasticity of materials with voids.

2. Basic equations

We refer the motion of a continuum to a fixed system of rectangular Cartesian axes $0x_k$ $(k = 1, 2, 3)$. We shall employ the usual summation and differentiation conventions: Latin subscripts are understood to range over integers $(1, 2, 3)$, summation over repeated subscripts is implied, subscripts preceded by a comma denote partial differentiation with respect to the corresponding Cartesian coordinate, and a superposed dot denotes time differentiation.

We consider a body that at time $t = 0$ occupies the bounded regular region B of Euclidean three-dimensional space whose boundary is the regular surface ∂B.

We assume that B is occupied by a mixture consisting of three components: an elastic solid, a viscous fluid and a gas. We use superscripts s, f, g to denote respectively, the elastic solid, the fluid and the gas. Let ρ_0^s, ρ_0^f and ρ_0^g denote the densities at time $t = 0$ of the three constituents, respectively. We consider the fundamental equations for mechanical behavior of the mixture in the framework of the linearized theory (see [4]). The equations of motion in the absence of the body forces are

$$\begin{aligned} t^s_{ji,j} + p^f_i + p^g_i &= \rho^s_0 \ddot{u}^s_i, \\ t^f_{ji,j} - p^f_i &= \rho^f_0 \ddot{u}^f_i, \\ t^g_{ji,j} - p^g_i &= \rho^g_0 \ddot{u}^g_i, \end{aligned} \tag{2.1}$$

where t^s_{ij}, t^f_{ij} and t^g_{ij} are the partial stress tensors, p^f_i and p^g_i are the internal body forces and u^s_i, u^f_i and u^g_i are the displacement vector fields.

The constitutive equations for a homogeneous and isotropic mixture are

$$\begin{aligned} t^s_{ij} &= \Big(-\sum_{a=f,g} \sigma^a e^a_{rr} + \lambda e^s_{rr}\Big)\delta_{ij} + 2\mu e^s_{ij}, \\ t^f_{ij} &= \Big(-\sigma^f e^s_{rr} - \sum_{a=f,g} \sigma^{fa} e^a_{rr} + \lambda_\nu \dot{e}^f_{rr}\Big)\delta_{ij} + 2\mu_\nu \dot{e}^f_{ij}, \\ t^g_{ij} &= \Big(-\sigma^g e^s_{rr} - \sum_{a=f,g} \sigma^{ga} e^a_{rr}\Big)\delta_{ij}, \\ p^a_i &= \sum_{b=f,g} \xi^{ab}(\dot{u}^b_i - \dot{u}^s_i), \quad a = f, g, \end{aligned} \tag{2.2}$$

where σ^a $(a = f, g)$, $\lambda, \mu, \sigma^{ab}$ $(a, b = f, g)$, $\lambda_\nu, \mu_\nu, \xi^{ab}$ $(a, b = f, g)$ are constitutive constants; δ_{ij} is the Kronecker delta; and e^s_{ij}, e^f_{ij} and e^g_{ij} are defined by

$$e^s_{ij} = \frac{1}{2}(u^s_{i,j} + u^s_{j,i}) \ , \quad e^f_{ij} = \frac{1}{2}(u^f_{i,j} + u^f_{j,i}) \ , \quad e^g_{ij} = \frac{1}{2}(u^g_{i,j} + u^g_{j,i}). \tag{2.3}$$

The coefficients in relation (2.2) have the following symmetries:

$$\sigma^{ab} = \sigma^{ba}, \ \xi^{ab} = \xi^{ba}, \ a, b = f, g. \tag{2.4}$$

To the system of field equations we adjoin boundary conditions and initial conditions. Many different types of boundary conditions are suggested in applications [8]–[11], [25]. We consider the following homogeneous boundary conditions:

$$\begin{gathered} u^s_i = 0, \qquad u^f_i = 0, \qquad u^g_i = 0 \qquad \text{on } \overline{S}_1 \times [0, \infty), \\ (t^s_{ji} + t^f_{ji} + t^g_{ji})n_j = 0, \ u^f_i - u^s_i = 0, \ u^g_i - u^s_i = 0 \quad \text{on } S_2 \times [0, \infty), \end{gathered} \tag{2.5}$$

where S_i $(i = 1, 2)$ are subsets of ∂B such that $\partial B = \overline{S}_1 \cup S_2$, $S_1 \cap S_2 = \emptyset$. Moreover, we adjoin the following initial conditions:

$$\begin{gathered} u^s_i(\mathbf{x}, 0) = a^s_i(\mathbf{x}) \ , \quad u^f_i(\mathbf{x}, 0) = a^f_i(\mathbf{x}) \ , \quad u^g_i(\mathbf{x}, 0) = a^g_i(\mathbf{x}), \\ \dot{u}^s_i(\mathbf{x}, 0) = b^s_i(\mathbf{x}) \ , \quad \dot{u}^f_i(\mathbf{x}, 0) = b^f_i(\mathbf{x}) \ , \quad \dot{u}^g_i(\mathbf{x}, 0) = b^g_i(\mathbf{x}), \quad \mathbf{x} \in B, \end{gathered} \tag{2.6}$$

where a^s_i, a^f_i, a^g_i, b^s_i, b^f_i, b^g_i are prescribed fields. We denote by $(\mathcal{P})$ the initial–boundary value problem defined by the basic equations (2.1), the constitutive equations (2.2), the geometrical equations (2.3), the boundary conditions (2.5) and the initial conditions (2.6).

As was shown by ERINGEN [4], the local form of the Clausius–Duhem inequality implies that

$$3\lambda_\nu + 2\mu_\nu \geq 0, \ \mu_\nu \geq 0, \tag{2.7}$$

and the following symmetric matrix is positive semi-definite

$$\Delta = \begin{pmatrix} \xi^{ff} & \xi^{fg} \\ \xi^{gf} & \xi^{gg} \end{pmatrix}, \tag{2.8}$$

so that the dissipation energy density Φ defined by

$$\Phi = \lambda_\nu \dot{e}^f_{ii} \dot{e}^f_{jj} + 2\mu_\nu \dot{e}^f_{ij} \dot{e}^f_{ij} + \sum_{a,b=f,g} \xi^{ab}(\dot{u}^a_i - \dot{u}^s_i)(\dot{u}^b_i - \dot{u}^s_i), \tag{2.9}$$

is non-negative.

The internal energy density $\mathcal{E}$ is defined by

$$\mathcal{E} = \frac{1}{2}\lambda e^s_{ii} e^s_{jj} + \mu e^s_{ij} e^s_{ij} - \sum_{a=f,g} \sigma^a e^a_{ii} e^s_{jj} - \frac{1}{2} \sum_{a,b=f,g} \sigma^{ab} e^a_{ii} e^b_{jj}. \tag{2.10}$$

3. Hypotheses and some preliminary results

Throughout this paper we shall assume the following:

(i) the densities ρ_0^s, ρ_0^f and ρ_0^g are strictly positive;

(ii) the following symmetric matrix is positive definite:

$$\delta = \begin{pmatrix} \lambda+2\mu & \lambda & \lambda & 0 & 0 & 0 & -\sigma^f & -\sigma^g \\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0 & -\sigma^f & -\sigma^g \\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0 & -\sigma^f & -\sigma^g \\ 0 & 0 & 0 & 2\mu & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mu & 0 & 0 \\ -\sigma^f & -\sigma^f & -\sigma^f & 0 & 0 & 0 & -\sigma^{ff} & -\sigma^{fg} \\ -\sigma^g & -\sigma^g & -\sigma^g & 0 & 0 & 0 & -\sigma^{fg} & -\sigma^{gg} \end{pmatrix}, \tag{3.1}$$

so, the internal energy density $\mathcal{E}$ defined by (2.10) is positive;

(iii) the symmetric matrix Δ is positive definite, that is we have

$$\xi_m \sum_{a=f,g} (\dot{u}_i^a - \dot{u}_i^s)(\dot{u}_i^a - \dot{u}_i^s) \leq \sum_{a=f,g} \xi^{ab}(\dot{u}_i^a - \dot{u}_i^s)(\dot{u}_i^b - \dot{u}_i^s) \leq \tag{3.2}$$

$$\leq \xi_M \sum_{a=f,g} (\dot{u}_i^a - \dot{u}_i^s)(\dot{u}_i^a - \dot{u}_i^s),$$

for any $\dot{u}_i^a - \dot{u}_i^s$, where $\xi_m > 0$ and $\xi_M > 0$ are the minimum and the maximum eigenvalues of ξ^{ab}, respectively.

Let us introduce the following energies:
the kinetic energy

$$\mathcal{K}(t) = \frac{1}{2} \int_B \Big(\sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(t) \dot{u}_i^\alpha(t) \Big) dv, \tag{3.3}$$

the internal energy

$$\mathcal{U}(t) = \int_B \mathcal{E}(t) dv, \tag{3.4}$$

the dissipation energy

$$\mathcal{D}(t) = \int_0^t \int_B \Phi(\tau) dv \, d\tau, \tag{3.5}$$

the total energy

$$E(t) = \mathcal{K}(t) + \mathcal{U}(t) + \mathcal{D}(t), \tag{3.6}$$

and

$$I(t) = \frac{1}{2}\int_B \Big(\sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(t) u_i^\alpha(t)\Big) dv + \frac{1}{2}\int_0^t\int_B \Big[\lambda_\nu e_{ii}^f(\tau) e_{jj}^f(\tau) + 2\mu_\nu e_{ij}^f(\tau) e_{ij}^f(\tau) + \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(\tau) - u_i^s(\tau)\Big)\Big(u_i^b(\tau) - u_i^s(\tau)\Big)\Big] dv\, d\tau. \tag{3.7}$$

Now, we recall some preliminary integral identities of Lagrange–Brun type [26], established in [14], that are essential in studying the temporal behavior of the solutions of the initial–boundary value problem $(\mathcal{P})$. For the readability of the paper we prefer to give here the proofs. Thus, in the present context, the lemmas 1,2 and 3 derived in [14] are:

LEMMA 1. (Conservation law of total energy). *For every* (u_i^s, u_i^f, u_i^g) *satisfying the equations of motion* (2.1), *the constitutive equations* (2.2) *and the geometrical equations* (2.3), *we have*

$$E(t) = E(0) + \int_0^t P(\tau,\tau) d\tau\,, \qquad t \in [0,\infty) \tag{3.8}$$

where

$$P(t,\tau) = \int_{\partial B} \Big(\sum_{\alpha=s,f,g} t_{ji}^\alpha(t) \dot{u}_i^\alpha(\tau)\Big) n_j\, da. \tag{3.9}$$

P r o o f. From the relations (2.2) and (2.10) it follows that

$$\sum_{\alpha=s,f,g} t_{ij}^\alpha \dot{e}_{ij}^\alpha = \frac{\partial \mathcal{E}}{\partial t} + \lambda_\nu \dot{e}_{ii}^f \dot{e}_{jj}^f + 2\mu_\nu \dot{e}_{ij}^f \dot{e}_{ij}^f. \tag{3.10}$$

On the other hand, in view of (2.1)–(2.3) we have

$$\sum_{\alpha=s,f,g} t_{ij}^\alpha \dot{e}_{ij}^\alpha = -\frac{1}{2}\frac{\partial}{\partial t}\Big(\sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha\Big) - \sum_{a,b=f,g} \xi^{ab}(\dot{u}_i^a - \dot{u}_i^s)(\dot{u}_i^b - \dot{u}_i^s) + \Big(\sum_{\alpha=s,f,g} t_{ji}^\alpha \dot{u}_i^\alpha\Big)_{,j}. \tag{3.11}$$

Then from the relations (3.10) and (3.11) we get

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha + \mathcal{E} + \int_0^t \Phi(\tau)d\tau\right) = \left(\sum_{\alpha=s,f,g} t_{ji}^\alpha \dot{u}_i^\alpha\right)_{,j}. \tag{3.12}$$

By an integration of the relation (3.12) over $B\times[0,t]$, and by using the divergence theorem and the relations (3.3)–(3.6) and (3.9), we obtain the identity (3.8) and the proof is complete.

LEMMA 2. *If* (u_i^s, u_i^f, u_i^g) *satisfies the relations* (2.1), (2.2) *and* (2.3), *then for every* $t\in[0,\infty)$

$$\frac{dI}{dt}(t) = \frac{dI}{dt}(0) + \int_0^t [4\mathcal{K}(\tau) + 2\mathcal{D}(\tau)]d\tau \tag{3.13}$$

$$- 2E(0)t - 2\int_0^t\int_0^\tau P(r,r)dr\,d\tau + \int_0^t \mathcal{W}(\tau,\tau)d\tau.$$

where

$$\mathcal{W}(t,\tau) = \int_{\partial B}\left(\sum_{\alpha=s,f,g} t_{ji}^\alpha(t)u_i^\alpha(\tau)\right)n_j\,da\,. \tag{3.14}$$

□

P r o o f. It follows from (2.2) and (2.10) that

$$\sum_{\alpha=s,f,g} t_{ij}^\alpha e_{ij}^\alpha = 2\mathcal{E} + \lambda_\nu \dot{e}_{ii}^f e_{jj}^f + 2\mu_\nu \dot{e}_{ij}^f e_{ij}^f. \tag{3.15}$$

By taking into account the relations (2.1)–(2.3) we obtain

$$\sum_{\alpha=s,f,g} t_{ij}^\alpha e_{ij}^\alpha = -\frac{\partial}{\partial t}\left(\sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha u_i^\alpha\right) - \sum_{a,b=f,g}\xi^{ab}(\dot{u}_i^a - \dot{u}_i^s)(u_i^b - u_i^s) \tag{3.16}$$

$$+ \sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha + \Big(\sum_{\alpha=s,f,g} t_{ji}^\alpha u_i^\alpha\Big)_{,j}.$$

Then the relations (3.15) and (3.16) imply

$$\frac{\partial}{\partial t}\left(\sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha u_i^\alpha\right) + \lambda_\nu \dot{e}_{ii}^f e_{jj}^f + 2\mu_\nu \dot{e}_{ij}^f e_{ij}^f \tag{3.17}$$

$$+ \sum_{a,b=f,g}\xi^{ab}(\dot{u}_i^a - \dot{u}_i^s)(u_i^b - u_i^s) = \sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha - 2\mathcal{E} + \left(\sum_{\alpha=s,f,g} t_{ji}^\alpha u_i^\alpha\right)_{,j}.$$

If we integrate relation (3.17) over $B \times [0,t]$ and use the divergence theorem and the relations (3.3), (3.4), (3.7) and (3.14), then we get

$$\frac{dI}{dt}(t) = \frac{dI}{dt}(0) + 2\int_0^t [\mathcal{K}(\tau) - \mathcal{U}(\tau)]d\tau + \int_0^t \mathcal{W}(\tau,\tau)d\tau. \tag{3.18}$$

A combination of the relations (3.8) and (3.18) gives the identity (3.13) and the proof is complete.

LEMMA 3. *For every* (u_i^s, u_i^f, u_i^g) *satisfying* (2.1) *to* (2.3), *the following identity holds*

$$\frac{dI}{dt}(t) = L(t) + \Lambda(t) + \frac{1}{2}\int_0^t [\mathcal{W}(t-\tau, t+\tau) - \mathcal{W}(t+\tau, t-\tau)]d\tau, \quad t > 0 \tag{3.19}$$

where

$$L(t) = \frac{1}{2}\int_B \left[\sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(0)\dot{u}_i^\alpha(2t) + \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^\alpha(2t) \right] dv, \tag{3.20}$$

and

$$\Lambda(t) = \frac{1}{2}\int_B \Big[\lambda_\nu e_{ii}^f(0) e_{jj}^f(2t) + 2\mu_\nu e_{ij}^f(0) e_{ij}^f(2t) + \sum_{a,b=f,g} \xi^{ab} \Big(u_i^a(0) - u_i^s(0) \Big) \Big(u_i^b(2t) - u_i^s(2t) \Big) \Big] dv. \tag{3.21}$$

□

P r o o f. Let us introduce the notation

$$R(t,\tau) = \sum_{\alpha=s,f,g} t_{ij}^\alpha(t) e_{ij}^\alpha(\tau). \tag{3.22}$$

Then, by (2.2) and (2.4), we obtain

$$\begin{aligned} R(t-\tau, t+\tau) - R(t+\tau, t-\tau) &= \lambda_\nu \dot{e}_{ii}^f(t-\tau) e_{jj}^f(t+\tau) \\ &+ 2\mu_\nu \dot{e}_{ij}^f(t-\tau) e_{ij}^f(t+\tau) - \lambda_\nu \dot{e}_{ii}^f(t+\tau) e_{jj}^f(t-\tau) - 2\mu_\nu \dot{e}_{ij}^f(t+\tau) e_{ij}^f(t-\tau) \\ &= -\frac{\partial}{\partial \tau}\Big(\lambda_\nu e_{ii}^f(t-\tau) e_{jj}^f(t+\tau) + 2\mu_\nu e_{ij}^f(t-\tau) e_{ij}^f(t+\tau) \Big). \end{aligned} \tag{3.23}$$

On the other hand, by means of the relations (2.1)–(2.3), we get

$$
\begin{aligned}
(3.24)\quad & R(t-\tau,t+\tau)-R(t+\tau,t-\tau) \\
&= \frac{\partial}{\partial\tau}\Big[\sum_{\alpha=s,f,g}\Big(\rho_0^\alpha \dot{u}_i^\alpha(t-\tau)u_i^\alpha(t+\tau)+\rho_0^\alpha u_i^\alpha(t-\tau)\dot{u}_i^\alpha(t+\tau)\Big)\Big] \\
&+ \frac{\partial}{\partial\tau}\Big[\sum_{a,b=f,g}\xi^{ab}\Big(u_i^a(t-\tau)-u_i^s(t-\tau)\Big)\Big(u_i^b(t+\tau)-u_i^s(t+\tau)\Big)\Big] \\
&+ \Big[\sum_{\alpha=s,f,g}\Big(t_{ji}^\alpha(t-\tau)u_i^\alpha(t+\tau)-t_{ji}^\alpha(t+\tau)u_i^\alpha(t-\tau)\Big)\Big]_{,j}.
\end{aligned}
$$

Further, from (3.23), we get

$$
\begin{aligned}
(3.25)\quad & \int_0^t\int_B [R(t-\tau,t+\tau)-R(t+\tau,t-\tau)]dv\,d\tau \\
&= -\int_B \Big[\lambda_\nu e_{ii}^f(0)e_{jj}^f(2t)+2\mu_\nu e_{ij}^f(0)e_{ij}^f(2t)\Big]dv \\
&+ \int_B \Big[\lambda_\nu e_{ii}^f(t)e_{jj}^f(t)+2\mu_\nu e_{ij}^f(t)e_{ij}^f(t)\Big]dv.
\end{aligned}
$$

From (3.14), (3.20) and (3.24) we deduce

$$
\begin{aligned}
(3.26)\quad & \int_0^t\int_B [R(t-\tau,t+\tau)-R(t+\tau,t-\tau)]dv\,d\tau \\
&= 2L(t)-2\int_B\Big(\sum_{\alpha=s,f,g}\rho_0^\alpha \dot{u}_i^\alpha(t)u_i^\alpha(t)\Big)dv \\
&+ \int_B\Big[\sum_{a,b=f,g}\xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(u_i^b(2t)-u_i^s(2t)\Big)\Big]dv \\
&- \int_B\Big[\sum_{a,b=f,g}\xi^{ab}\Big(u_i^a(t)-u_i^s(t)\Big)\Big(u_i^b(t)-u_i^s(t)\Big)\Big]dv \\
&+ \int_0^t [\mathcal{W}(t-\tau,t+\tau)-\mathcal{W}(t+\tau,t-\tau)]d\tau.
\end{aligned}
$$

A combination of the relations (3.25) and (3.26) implies the desired result. □

4. Cesàro means and the asymptotic partition

In this section we study the time asymptotic behavior of the solutions of the problem $(\mathcal{P})$ defined by the relations (2.1) to (2.6). To this end, we introduce the Cesàro means of various parts of the total energy and then, using the identities (3.8), (3.13) and (3.19), we establish the relations that describe the asymptotic behavior of the mean energies.

If (u_i^s, u_i^f, u_i^g) is a solution for the problem $(\mathcal{P})$, then we introduce the Cesàro means

$$\mathcal{K}_C(t) := \frac{1}{t}\int_0^t \mathcal{K}(\tau)d\tau \ , \tag{4.1}$$

$$\mathcal{U}_C(t) := \frac{1}{t}\int_0^t \mathcal{U}(\tau)d\tau \ , \tag{4.2}$$

$$\mathcal{D}_C(t) := \frac{1}{t}\int_0^t \mathcal{D}(\tau)d\tau \ . \tag{4.3}$$

If meas $S_1 = 0$, where meas S represents the area $\int_S da$ of the surface S. Then there exists a family of rigid motions ($u_i^s = u_i^f = u_i^g = c_i + \varepsilon_{ijk}x_j d_k$, c_i, d_i – constants, ε_{ijk} – alternating symbol) that satisfy equations of motion (2.1), constitutive equations (2.2) and the boundary conditions (2.5). For this reason, we decompose the initial data a_i^s and b_i^s as

$$a_i^s = a_i^{\star s} + U_i^{0s} \ , \qquad b_i^s = b_i^{\star s} + V_i^{0s} \ , \tag{4.4}$$

where $a_i^{\star s}$ and $b_i^{\star s}$ are rigid displacements determined in such a way that

$$\int_B \rho_0^s U_i^{0s} dv = 0 \ , \qquad \int_B \rho_0^s \varepsilon_{ijk} x_j U_k^{0s} dv = 0 \ , \tag{4.5}$$

$$\int_B \rho_0^s V_i^{0s} dv = 0 \ , \qquad \int_B \rho_0^s \varepsilon_{ijk} x_j V_k^{0s} dv = 0 \ .$$

We consider the sets

$$\hat{\mathbf{C}}^1(B) := \{\mathbf{v} = (v_1, v_2, v_3), v_i \in C^1(\overline{B}) : v_i = 0 \text{ on } S_1 \text{ and if meas } S_1 = 0 \ ,$$

$$\text{then } \int_B \rho_0^s v_i dv = 0 \ , \qquad \int_B \rho_0^s \varepsilon_{ijk} x_j v_k dv = 0 \ \}.$$

$\hat{\mathbf{W}}_1(B)$:=the completion of $\hat{\mathbf{C}}^1(\mathrm{B})$ by means of $||\cdot||_{\mathbf{W}_1(B)}$ where $C^1(\overline{B})$ represents the set of scalar functions that are continuous and continuously differentiable on $\overline{B}$. Moreover $\mathbf{W}_m(B) := [W_m(B)]^3$, where $W_m(B)$ is the familiar Sobolev space (see [27]).

The hypothesis (ii) assures that the following inequality [28] holds:

$$\int_B [\lambda v_{i,i} v_{j,j} + \frac{\mu}{2}(v_{i,j} + v_{j,i})(v_{i,j} + v_{j,i})]dv \geq m_1 \int_B v_i v_i dv \,, \tag{4.6}$$

$$m_1 = \text{const} > 0 \,, \qquad \forall\, \mathbf{v} \in \hat{\mathbf{W}}_1(\mathbf{B}) \,.$$

If meas $S_1 = 0$, then we shall find it is a convenient practice to decompose the solution (u_i^s, u_i^f, u_i^g) in the form

$$u_i^s = a_i^{\star s} + t b_i^{\star s} + v_i^s, \quad u_i^f = a_i^{\star s} + t b_i^{\star s} + v_i^f, \quad u_i^g = a_i^{\star s} + t b_i^{\star s} + v_i^g, \tag{4.7}$$

where $(\mathbf{v^s}, \mathbf{v^f}, \mathbf{v^g}) \in \hat{\mathbf{W}}_1(\mathbf{B}) \times \mathbf{W}_1(\mathbf{B}) \times \mathbf{W}_1(\mathbf{B})$ represents the solution of the initial boundary value problem $(\mathcal{P})$ in which the initial conditions are substituted by

$$\begin{gathered} v_i^s = U_i^{0s}, \qquad v_i^f = a_i^f - a_i^{\star s}, \qquad v_i^g = a_i^g - a_i^{\star s}, \\ \dot{v}_i^s = V_i^{0s}, \qquad \dot{v}_i^f = b_i^f - b_i^{\star s}, \qquad \dot{v}_i^g = b_i^g - b_i^{\star s}, \text{ on } B, \ t = 0. \end{gathered} \tag{4.8}$$

We are now ready to derive the asymptotic partition of the energies.

THEOREM 1. *Let (u_i^s, u_i^f, u_i^g) be a solution of the initial boundary value problem $(\mathcal{P})$. Then, for all choices of initial data $\mathbf{a^s}$, $\mathbf{a^f}$, $\mathbf{a^g}$, $\mathbf{b^f} \in \mathbf{W_1(B)}$, $\mathbf{b^s}$, $\mathbf{b^g} \in \mathbf{W_0(B)}$, we have:*

$1)^0$ *if* meas $S_1 \neq 0$, *then*

$$\lim_{t\to\infty} \mathcal{K}_C(t) = \lim_{t\to\infty} \mathcal{U}_C(t), \tag{4.9}$$

$$\lim_{t\to\infty} \mathcal{D}_C(t) = E(0) - 2\lim_{t\to\infty} \mathcal{K}_C(t) = E(0) - 2\lim_{t\to\infty} \mathcal{U}_C(t). \tag{4.10}$$

$2)^0$ *if* meas $S_1 = 0$, *then*

$$\lim_{t\to\infty} \mathcal{K}_C(t) = \lim_{t\to\infty} \mathcal{U}_C(t) + \frac{1}{2}\int_B (\rho_0^s b_i^{\star s} b_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a b_i^{\star s}) dv, \tag{4.11}$$

$$\begin{aligned} \lim_{t\to\infty} \mathcal{D}_C(t) &= E(0) - 2\lim_{t\to\infty} \mathcal{K}_C(t) + \frac{1}{2}\int_B (\rho_0^s b_i^{\star s} b_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a b_i^{\star s}) dv \\ &= E(0) - 2\lim_{t\to\infty} \mathcal{U}_C(t) - \frac{1}{2}\int_B (\rho_0^s b_i^{\star s} b_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a b_i^{\star s}) dv. \end{aligned} \tag{4.12}$$

P r o o f. By taking into account the fact that (u_i^s, u_i^f, u_i^g) is the solution of the problem $(\mathcal{P})$, from (3.8), we deduce

$$\mathcal{K}(t) + \mathcal{U}(t) + \mathcal{D}(t) = E(0), \qquad t \leq 0. \tag{4.13}$$

If we further use the relations (3.13) and (3.19), we get

$$\int_0^t [4\mathcal{K}(\tau) + 2\mathcal{D}(\tau)]d\tau = 2E(0)t + \Lambda(t) + \Gamma(t) - \frac{dI}{dt}(0), \qquad t \geq 0. \tag{4.14}$$

A combination of the relations (4.13) and (4.14) leads to the identity

$$\mathcal{K}_C(t) - \mathcal{U}_C(t) = \frac{1}{2t}\left[\Lambda(t) + \Gamma(t) - \frac{dI}{dt}(0)\right]. \tag{4.15}$$

By letting t tend to infinity and making use of the relations (3.20) and (3.21), we obtain

$$\begin{aligned}\lim_{t\to\infty}[\mathcal{K}_C(t) - \mathcal{U}_C(t)] = \lim_{t\to\infty}\frac{1}{4t}\int_B \Big\{ &\sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(0)\dot{u}_i^\alpha(2t) \\ &+ \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0)u_i^\alpha(2t) + \lambda_\nu e_{ii}^f(0)e_{jj}^f(2t) + 2\mu_\nu e_{ij}^f(0)e_{ij}^f(2t) \\ &+ \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0) - u_i^s(0)\Big)\Big(u_i^b(2t) - u_i^s(2t)\Big)\Big\}dv.\end{aligned} \tag{4.16}$$

On the basis of the hypotheses (i)–(iii), relations (2.7), (3.3)–(3.5), (4.13) and Schwarz's inequality, we deduce for the terms in the right-hand side of (4.16) the following estimates:

$$\begin{aligned}\int_B \sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(0)\dot{u}_i^\alpha(2t)dv &\leq \left(\int_B \sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(0)u_i^\alpha(0)dv\right)^{1/2} \\ &\quad \times \left(\int_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(2t)\dot{u}_i^\alpha(2t)dv\right)^{1/2} \\ &\leq \sqrt{2E(0)}\left(\int_B \sum_{\alpha=s,f,g} \rho_0^\alpha u_i^\alpha(0)u_i^\alpha(0)dv\right)^{1/2};\end{aligned} \tag{4.17}$$

$$(4.18)\quad \int_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^\alpha(2t)\,dv = \int_B \Big\{ \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^s(2t)$$

$$+ \int_0^{2t} \sum_{a=f,g} \rho_0^a \dot{u}_i^a(0)[\dot{u}_i^a(\tau) - \dot{u}_i^s(\tau)]\,d\tau + \sum_{a=f,g} \rho_0^a \dot{u}_i^a(0)[u_i^a(0) - u_i^s(0)] \Big\} dv$$

$$\le \int_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^s(2t)\,dv + \Big(\int_0^{2t}\int_B \sum_{a=f,g} \frac{(\rho_0^a)^2}{\xi_m} \dot{u}_i^a(0)\dot{u}_i^a(0)\,dv\,d\tau \Big)^{1/2}$$

$$\times \Big(\int_0^{2t}\int_B \sum_{a,b=f,g} \xi^{ab}[\dot{u}_i^a(\tau) - \dot{u}_i^s(\tau)][\dot{u}_i^b(\tau) - \dot{u}_i^s(\tau)]\,dv\,d\tau \Big)^{1/2}$$

$$+ \int_B \sum_{a=f,g} \rho_0^a \dot{u}_i^a(0)[u_i^a(0) - u_i^s(0)]\,dv \le \int_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^s(2t)\,dv$$

$$+ \sqrt{2tE(0)} \Big(\int_B \sum_{a=f,g} \frac{(\rho_0^a)^2}{\xi_m} \dot{u}_i^a(0)\dot{u}_i^a(0)\,dv \Big)^{1/2}$$

$$+ \int_B \sum_{a=f,g} \rho_0^a \dot{u}_i^a(0)[u_i^a(0) - u_i^s(0)]\,dv;$$

$$(4.19)\quad \int_B [\lambda_\nu e_{ii}^f(0) e_{jj}^f(2t) + 2\mu_\nu e_{ij}^f(0) e_{ij}^f(2t)]\,dv = \int_0^{2t}\int_B [\lambda_\nu e_{ii}^f(0)\dot{e}_{jj}^f(\tau)$$

$$+ 2\mu_\nu e_{ij}^f(0)\dot{e}_{ij}^f(\tau)]\,dv\,d\tau + \int_B [\lambda_\nu e_{ii}^f(0) e_{jj}^f(0) + 2\mu_\nu e_{ij}^f(0) e_{ij}^f(0)]\,dv$$

$$\le \sqrt{2tE(0)} \Big(\int_B [\lambda_\nu e_{ii}^f(0) e_{jj}^f(0) + 2\mu_\nu e_{ij}^f(0) e_{ij}^f(0)]\,dv \Big)^{1/2}$$

$$+ \int_B [\lambda_\nu e_{ii}^f(0) e_{jj}^f(0) + 2\mu_\nu e_{ij}^f(0) e_{ij}^f(0)]\,dv;$$

$$(4.20)\quad \int\limits_B \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(u_i^b(2t)-u_i^s(2t)\Big)dv$$

$$= \int\limits_0^{2t}\int\limits_B \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(\dot{u}_i^b(\tau)-\dot{u}_i^s(\tau)\Big)dv\ d\tau$$

$$+ \int\limits_B \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(u_i^b(0)-u_i^s(0)\Big)dv$$

$$\leq \sqrt{2tE(0)}\left(\int\limits_B \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(u_i^b(0)-u_i^s(0)\Big)dv\right)^{1/2}$$

$$+ \int\limits_B \sum_{a,b=f,g} \xi^{ab}\Big(u_i^a(0)-u_i^s(0)\Big)\Big(u_i^b(0)-u_i^s(0)\Big)dv.$$

Using the estimates (4.17)–(4.20) in (4.16) we obtain

$$(4.21)\quad \lim_{t\to\infty}[\mathcal{K}_C(t)-\mathcal{U}_C(t)] = \lim_{t\to\infty}\frac{1}{4t}\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0)u_i^s(2t)dv.$$

Let us first consider $1)^0$. Since meas $S_1 \neq 0$ and $\mathbf{u^s} \in \hat{\mathbf{W}}_\mathbf{1}(\mathbf{B})$, from (2.10), (3.4), (3.6), (4.6) and (4.13), we deduce

$$(4.22)\quad \int\limits_B u_i^s(\tau)u_i^s(\tau)dv \leq \frac{1}{m_1}\int\limits_B 2\mathcal{E}(\tau)dv \leq \frac{2}{m_1}E(0)\ ,$$

so, by means of the Schwarz inequality, we get

$$(4.23)\quad \lim_{t\to\infty}\frac{1}{4t}\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0)u_i^s(2t)dv = 0.$$

Thus, the relations (4.21) and (4.23) give the relation (4.9). A combination of the relations (4.9) and (4.13) give the relation (4.10).

Let us consider $2)^0$. Using the decomposition (4.4) and (4.7), we have

$$(4.24)\quad \frac{1}{4t}\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^s(2t)dv$$

$$= \frac{1}{4t}\int\limits_B \Big[\rho_0^s(b_i^{\star s} + V_i^{0s}) + \sum_{a=f,g} \rho_0^a b_i^a\Big]\Big[a_i^{\star s} + 2tb_i^{\star s} + v_i^s(2t)\Big]dv$$

$$= \frac{1}{4t}\int\limits_B \Big[\rho_0^s b_i^{\star s} a_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a a_i^{\star s}\Big]dv + \frac{1}{4t}\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha b_i^\alpha v_i^s(2t)dv$$

$$+ \frac{1}{2}\int\limits_B \Big[\rho_0^s b_i^{\star s} b_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a b_i^{\star s}\Big]dv.$$

The Korn inequality (4.6) and the relations (2.10), (3.4) and (4.13) imply

$$(4.25)\quad \int\limits_B v_i^s(\tau) v_i^s(\tau)dv \le \frac{1}{m_1}\int\limits_B 2\mathcal{E}(\tau)dv \le \frac{2}{m_1}E(0)\ ,$$

so, by means of the Schwarz inequality, we deduce

$$(4.26)\quad \lim_{t\to\infty}\frac{1}{4t}\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha \dot{u}_i^\alpha(0) u_i^s(2t)dv = \frac{1}{2}\int\limits_B \Big[\rho_0^s b_i^{\star s} b_i^{\star s} + \sum_{a=f,g} \rho_0^a b_i^a b_i^{\star s}\Big]dv\ .$$

Thus, using (4.26) from (4.21) we obtain (4.11). The relation (4.12) follows then by coupling the relations (4.11) and (4.13). The proof is complete. □

REMARK 1. Relations (4.9) and (4.11) (restricted to the class of initial data for which $b_i^{\star s} = 0$) prove the asymptotic equipartition of the mean kinetic and internal energies.

REMARK 2. Similarly to the previous papers concerning asymptotic partition of energy, we supposed that body forces are absent ($f_i^s = f_i^f = f_i^g = 0$) and this assumption is essential in our analysis. Generally, the asymptotic partition of energy will be modified by the presence of body forces. For a solution (u_i^s, u_i^f, u_i^g) of the problem $(\mathcal{P})$ the relation (4.13) becomes

$$(4.13)'\quad \mathcal{K}(t) + \mathcal{U}(t) + \mathcal{D}(t) = E(0) + \int\limits_0^t\int\limits_B \sum_{\alpha=s,f,g} \rho_0^\alpha f_i^\alpha(\tau)\dot{u}_i^\alpha(\tau)dvd\tau, \quad t \le 0$$

and it leads to estimate terms like that in the right-hand side of (4.16). Our analysis in the above can be applied under appropriate assumptions concerning the behavior of the forces at infinity, but the calculation becomes more complicated.

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Pure shear of a cubic crystal

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LARGE SIMPLE shear of a crystal of cubic symmetry is considered. The equations of second order elasticity theory are applied. In this approximation three constants of the second order and six constants of the third order characterize the crystal. The stress for three shearing planes and three directions for each plane has been calculated. The stresses have been calculated separately for each material constant. For copper, the shearing planes and shearing directions for which stress reaches extreme values have been determined. The extreme values for each component of the traction have been calculated.

1. Introduction

CRYSTALS ARE of special interest in fundamental research. Taking into account the symmetries (called point groups) the crystals may be divided into 32 classes. All crystals belonging to one class have the same macroscopic symmetry. Cubic crystals possess the highest symmetry. Their mechanical behavior in the linear case is described by three elastic constants. Triclinic crystals belong to the class of the lowest symmetry. In the linear case they are described by twenty-one elastic constants.

Isotropic materials possess higher symmetry. Mechanical properties of linear isotropic material may be described by two elastic constants only. Isotropic crystals do not exist. Typical isotropic material is an amorphous material, e.g. glass. Approximation of an isotropic material is a polycrystalline cluster of randomly oriented crystals. Most of the experience in engineering is connected with isotropic materials. Manufactured pieces of single crystals are frequently used in physical experiments and physical equipment.

External load applied to a crystal results in a deformation. Since a crystal is not isotropic, its stress field differs from that of an isotropic material. The present paper aims at analysis of the forces, necessary to result in a shearing given in advance.

All 32 symmetry groups may be analyzed for linear and for the nonlinear material. Obviously a linear material, due to simplicity, is of special interest. Nonlinearity is manifested in the additional phenomena. Trying to avoid com-

plex, non-transparent considerations, we do not consider general elasticity, but confine ourselves to the second-order theory. The second order theory of elasticity was presented in the monograph of GREEN and ADKINS [1]. All equations of the first chapter are based on [1]. We confine the analysis to one symmetry only, namely to the cubic symmetry. Typical material of this symmetry is the crystal of copper.

Common for all theories is the notion of the strain tensor. Introduce the Cartesian coordinates x_j. The material point of the body is identified by its position x_j in the stress-free initial state. In the course of time, the point x_j moves to a new position. The displacement vector u_i is a function of the Cartesian coordinates x_j and time $t, u_i = u_i(x_j, t)$. In the whole paper we compare two states only and time serves only as a parameter. Therefore for simplicity we shall write $u_i = u_i(x_j)$. Partial derivative of $u_i(x_j)$ with respect to x_j is the displacement gradient $u_{i,j}$. The strain tensor ε_{ij} may be expressed by the displacement gradient, [1]

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,i} + u_{j,i} + u_{r,i}\, u_{r,j}). \tag{1.1}$$

The nonlinear product $u_{r,i}\, u_{r,j}$ is present in this expression. Therefore the deformation tensor ε_{ij} is always a nonlinear function of the displacement gradient. The linear measure of strain disregarding this term may be used only in the linear theory, where the stress is a linear function of strain.

The relation (1.1) is purely geometrical. No material properties are involved. The elastic energy (strain energy) is a nonlinear function of strain ε_{ij}. Second order elasticity is the simplest generalization of the linear elasticity. The expression for the elastic energy Φ (per unit volume in the stress-free state) takes into account the cubes, but neglects the fourth higher powers of strain tensor ε_{ij}. The elastic energy Φ reads

$$\Phi = \frac{1}{2} c_{ijkm}\, \varepsilon_{ij}\, \varepsilon_{km} + \frac{1}{6} c_{ijkmrs}\, \varepsilon_{ij}\, \varepsilon_{km}\, \varepsilon_{rs}. \tag{1.2}$$

It is a cubic function of strain, but polynomial of the sixth order in the displacement gradient. The coefficients 1/2 and 1/6 are commonly accepted in the literature, [2].

Summation convention is accepted in the whole present paper. The tensor c_{ijkm} is the tensor of second order elastic constants and c_{ijkmrs} is the tensor of third order elastic constants. In some older papers these tensors are called first and second order elastic constants, respectively. Since the expression (1.1) is homogeneous in ε_{ij} it may be assumed that $c_{ijkm} = c_{kmij}$ and $c_{ijkmrs} = c_{kmijrs} = c_{ijrskm}$. Since ε_{ij} is symmetric, it may be assumed without loosing the generality that the constants satisfy the relations $c_{ijkm} = c_{jikm}$ and $c_{ijkmrs} = c_{jikmrs}$.

The elastic constants of the second order and of the third order may be therefore assumed to posses the following symmetries

$$c_{ijkm} = c_{kmij} = c_{jikm}, \tag{1.3}$$

$$c_{ijkmrs} = c_{kmijrs} = c_{ijrskm} = c_{jirskm}. \tag{1.4}$$

Symmetry of the crystal results in additional symmetries. As mentioned above, the second order elastic constants c_{ijkm} for triclinic symmetry may be expressed by 21 independent material constants. In the simplest case of cubic symmetry there are only 3 non-zero independent constants of the second order and 6 material constants of the third order. The 81 constants c_{ijkm} and 729 constants c_{ijkmrs} may therefore for the cubic crystal be expressed by only 9 elastic constants. The isotropic material is characterized by only 5 elastic constants, namely 2 constants of second order (Lamé constants) and 3 constants of third order.

There exist at least eight different methods of measuring the constants of the third order. The measurement of forces in static deformation is one of them, but the most frequently used method is based on measurements of the ultrasonic wave speeds.

Denote by H_{ij} the symmetrized derivative of the elastic energy Φ with respect to the deformation ε_{ij}

$$H_{ij} = \frac{\partial \Phi}{\partial \varepsilon_{ij}} + \frac{\partial \Phi}{\partial \varepsilon_{ji}}. \tag{1.5}$$

From (1.2) and the symmetries (1.3)–(1.4) there follows

$$\frac{\partial \Phi}{\partial \varepsilon_{ij}} = c_{ijkm}\,\varepsilon_{km} + \frac{1}{2} c_{ijkmrs}\,\varepsilon_{km}\,\varepsilon_{rs}, \tag{1.6}$$

and further

$$H_{ij} = 2c_{ijkm}\varepsilon_{km} + c_{ijkmrs}\,\varepsilon_{km}\,\varepsilon_{rs}. \tag{1.7}$$

The stress tensor τ_{ij} may be expressed by the function H_{ij} and the displacement gradient $u_{i,j}$

$$2\tau_{ij} = H_{ij} + H_{ir} u_{j,r}. \tag{1.8}$$

The stress tensor τ_{ij} is not symmetric. It is in fact the first Piola-Kirchhoff stress tensor. This tensor may be expressed by the deformation gradient and material constants. Full expression for τ_{ij} will be given further for simple shear.

The most important mechanism of deformation of a crystal is simple shear, [4]. This deformation induces relatively small change of the volume. Consider simple shear of a crystal of arbitrary symmetry. Denote by n_i the normal to the shearing plane and by k_i the shearing direction. Both vectors are unit vectors and orthogonal to each other

$$k_i k_i = 1, \quad n_i n_i = 1, \quad k_i n_i = 0. \tag{1.9}$$

In the case of shear in the direction k_i, the displacement vector u_i has the direction of k_i and is proportional to the distance $n_r x_r$ from the plane $n_r x_r$=0. The displacement u_i for hear reads

$$u_i(x_r) = \nu k_i n_r x_r, \tag{1.10}$$

where ν is the measure of shear. For the whole plane $n_r x_r$=const the displacement vector is the same. The strain tensor ε_{ij} may now be calculated from (1.1) and (1.10). For each material, linear and nonlinear, it consists of a term proportional to ν and a term proportional to ν^2

$$2\varepsilon_{ij} = \nu\left(k_i n_j + k_j n_i\right) + \nu^2 n_i n_j. \tag{1.11}$$

Substitute the above expression into (1.8) and take into account the symmetries of c_{ijkm} and c_{ijkmrs} to obtain the following expression for the stress tensor:

$$\tau_{ij} = \nu c_{ijpq} k_p n_q + \nu^2 \left(\frac{1}{2} c_{ijpqrs} k_p k_r n_q n_s + \frac{1}{2} c_{ijpq} n_p n_q + c_{impq} k_j k_p n_m n_q\right). \tag{1.12}$$

The stress tensor is uniquely determined by the strain energy Φ and the shear. In (1.12) the terms of the order ν^3 have been neglected, since already Φ does not take into account the third powers of ε_{ij}. The stress vector t_i acting on a surface with unit normal n_i equals the product of the stress tensor τ_{ij} and the vector n_i

$$t_j = \nu c_{ijpq} k_p n_i n_q + \nu^2 \left(\frac{1}{2} c_{ijpqrs} k_p k_r n_i n_q n_s + \frac{1}{2} c_{ijpq} n_i n_p n_q + k_j c_{impq} k_p n_i n_m n_q\right). \tag{1.13}$$

In general this vector is neither perpendicular, nor collinear with k_i or n_i. The component of t_j in the shear direction k_i equals $t_j k_j$. Define the vector b_i as the vector product of k_i and n_i

$$b_i = \varepsilon_{irs} k_r n_s, \tag{1.14}$$

where ε_{irs} is the permutation symbol. This unit vector is orthogonal to k_i and n_i.

Define three components s_k, s_n, s_b of the stress vector as the scalar products of the stress vector and the unit vectors k_i, n_i, and b_i

$$s_k = t_j k_j, \quad s_n = t_j n_j, \quad s_b = t_j b_j. \tag{1.15}$$

In accord with the above relations there hold the relations

$$\begin{aligned} s_k &= \nu s_{k1} + \nu^2 (s_{k2} + s_{k3}), \\ s_n &= \nu s_{n1} + \nu^2 (s_{n2} + s_{n3}), \\ s_b &= \nu s_{b1} + \nu^2 (s_{b2} + s_{b3}), \end{aligned} \tag{1.16}$$

where

$$\begin{aligned} s_{k1} &= c_{ijpq} k_i n_j k_p n_q, \\ s_{k2} &= \frac{3}{2} c_{ijpq} k_i n_j k_p n_q, \\ s_{k3} &= \frac{1}{2} c_{ijpqrs} k_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.17}$$

$$\begin{aligned} s_{n1} &= c_{ijpq} n_i n_j k_p n_q, \\ s_{n2} &= \frac{1}{2} c_{ijpq} n_i n_j n_p n_q, \\ s_{n3} &= \frac{1}{2} c_{ijpqrs} n_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.18}$$

$$\begin{aligned} s_{b1} &= c_{ijpq} b_i n_j k_p n_q, \\ s_{b2} &= \frac{3}{2} c_{ijpq} b_i n_j k_p n_q, \\ s_{b3} &= \frac{1}{2} c_{ijpqrs} b_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.19}$$

The projections of t_i on n_i and on b_i , i.e. the scalar products $t_i n_i$ and $t_i b_i$ in linear elasticity of isotropic material are equal to zero. In nonlinear elasticity the projection of t_i on n_i is different from zero, even for isotropic material. In fact this stress component for isotropic material is always negative. For anisotropic material both projections are in general different from zero. The parameter s_k

introduced above is a measure of the projection of the stress vector on the direction k_i.

Each of the expressions for s_k, s_n, s_b consists of a part proportional to the amount of shear ν and a part proportional to the squared amount of shear ν^2. The parts s_{k1}, s_{n1}, s_{b1} do not take into account the nonlinearity and are exactly the same as in linear elasticity. The other parts take into account nonlinearity. More exactly, the other parts express the second term of the Taylor expansion of stress vector t_i. For infinitesimal shear ν the first terms s_{k1}, s_{n1}, s_{b1} in (1.17)–(1.19) are the leading terms. For other ν the second and third terms must be taken into account. In the next chapter we analyze separately the terms of (1.16)–(1.18).

Shear stiffness s equals the ratio of the component of t_j in the shear direction k_j and the measure of shear ν. Stiffness is equal to the sum

$$s = s_{k1} + \nu(s_{k2} + s_{k3}). \tag{1.20}$$

2. Linear elasticity

Analysis of the present chapter is based on the principal terms of s_{k1}, s_{n1}, s_{b1}, namely on the relations

$$\begin{aligned} s_{k1} &= c_{ijpq} k_i n_j k_p n_q, \\ s_{n1} &= c_{ijpq} n_i n_j k_p n_q, \\ s_{b1} &= c_{ijpq} b_i n_j k_p n_q. \end{aligned} \tag{2.1}$$

Since b_i as the vector product of n_i and k_i may be expressed by n_i and k_i, the above functions depend on n_i and k_i only. Note that s_{k1} is an even function of n_i and k_i; s_{n1} is an odd function of n_i and an odd function of k_i; finally s_{b1} is an odd function of n_i and even function of k_i.

In the present paper we consider only one definite material symmetry, namely the cubic symmetry. Other crystal symmetries may be treated in the same way. In the linear theory there exist only three independent elastic constants of cubic crystal. In abbreviated notation ($\varepsilon_1 = \varepsilon_{11}$, $\varepsilon_2 = \varepsilon_{22}$, ..., $\varepsilon_4 = 2\varepsilon_{23}$, etc.) they are h_{11}, h_{12} and h_{44} , cf. [2]. All 81 components of the elastic constants tensor c_{ijpq} may be expressed by the three constants h_{11}, h_{12} and h_{44}, namely

$$\begin{aligned} &c_{1111} = c_{2222} = c_{3333} = h_{11}, \\ &c_{1122} = c_{1133} = c_{2233} = c_{2211} = c_{3311} = c_{3322} = h_{12}, \\ &c_{2323} = c_{2332} = c_{3223} = \ldots = c_{1212} = c_{1221} = h_{44}. \end{aligned} \tag{2.2}$$

The remaining components of the tensor c_{ijpq} (elastic constants of the second order), e.g. the components c_{1231}, c_{1112}, are equal zero.

In order to gain better recognition of the stresses in this chapter we do not consider any specified real material, but aim to analyze the influence of elastic constants on stress in pure shear of cubic crystal. This fact suggests separate consideration of three cases: i) $h_{11} = 1$, $h_{12} = 0$, $h_{44} = 0$, ii) $h_{11} = 0$, $h_{12} = 1$, $h_{44} = 0$ and iii) $h_{11} = 0$, $h_{12} = 0$, $h_{44} = 1$.

Calculate the coefficients s_{k2}, s_{n2} and s_{b2} for three different shear planes (1,0,0), (1,1,0) and (1,1,1). For each shear plane three shearing planes were selected.

Consider first the shearing plane n_i=(1,0,0) and three different shearing directions

$$k_i^{(1)} = (0,1,0), \quad k_i^{(2)} = (0,1,1), \quad k_i^{(3)} = (0,1,1+\sqrt{2}). \tag{2.3}$$

The vector $k_i^{(3)} = (0,1,1+\sqrt{2})$ bisects the angle between the first two. Because of the symmetry of the problem, the values of s_{k2}, s_{n2} and s_{b2} for the directions $k_i^{(1)}$ and $k_i^{(2)}$ take extreme values.

The shearing plane n_i=(1,1,0) is equally inclined to the directions (1,0,0) and (0,1,0) and parallel to the direction (0,0,1). Three shearing directions

$$k_i^{(4)} = (1,-1,0), \quad k_i^{(5)} = (0,0,1), \quad k_i^{(6)} = (1,-1,\sqrt{2}) \tag{2.4}$$

are orthogonal to (1,1,0). The shearing directions $k_i^{(4)}$=(1,–1,0) and $k_i^{(5)}$ =(0,0,1) are the geometrical symmetry directions of the problem. The shearing direction $k_i^{(6)}$= (1,–1,$\sqrt{2}$) bisects the shearing directions $k_i^{(4)}$ and $k_i^{(5)}$.

The shearing plane n_i=(1,1,1) is equally inclined to the three directions (1,0,0), (0,1,0) and (0,0,1). The proposed shearing directions are

$$k_i^{(7)} = (2,-1,-1), \quad k_i^{(8)} = (1,-1,0), \quad k_i^{(9)} = (2+\sqrt{3},-1-\sqrt{3},-1). \tag{2.5}$$

The shearing directions $k_i^{(7)}$=(2,–1,–1) and $k_i^{(8)}$=(1,–1,0) are the symmetry directions of the problem. Direction (1,–2,1) is equivalent to the direction (2,–1,–1). Since (1,–1,0) bisects the directions (1,–2,1) and (2,–1,–1), it is a symmetry direction of the problem. The direction $k_i^{(9)}$ = (2+$\sqrt{3}$,–1–$\sqrt{3}$,–1) bisects the directions k_i =(1,–1,0) and k_i =(2,–1,–1).

The vectors $k_i^{(1)}$, $k_i^{(2)}$, ..., $k_i^{(9)}$ and the corresponding shearing planes are listed in the first two columns of Table 1. In calculation, one of the elastic constants was assumed to be equal 1, the other two to be equal zero.The following values s_{k1}, s_{n1} and s_{b1} were calculated.

The values given in the first two columns are the components of the vector parallel to n_i and the vector parallel to k_i. In computations they must be normalized to obtain the vectors n_i and k_i of unit length. For the shearing plane

Table 1. Coefficients s_{k1}, s_{n1}, s_{b1} for copper.

n_i	k_i	h_{11}=1, h_{12}=0, h_{44}=0			h_{11}=0, h_{12}=1, h_{44}=0			h_{11}=0, h_{12}=0, h_{44}=1		
		s_{k1}	s_{n1}	s_{b1}	s_{k1}	s_{n1}	S_{b1}	s_{k1}	s_{n1}	s_{b1}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	0	0	1	0	0
	$k_i^{(2)}$	0	0	0	0	0	0	1	0	0
	$k_i^{(3)}$	0	0	0	0	0	0	1	0	0
(1,1,0)	$k_i^{(4)}$	.500	0	0	−.500	0	0	0	0	0
	$k_i^{(5)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(6)}$	.250	0	−.250	−.250	0	.250	.500	0	.500
(1,1,1)	$k_i^{(7)}$	.333	0	0	−.333	0	0	.333	0	0
	$k_i^{(8)}$	.333	0	0	−.333	0	0	.333	0	0
	$k_i^{(9)}$	.333	0	0	−.333	0	0	.333	0	0

Table 2. Coefficients s_{n2} for n_i=(1,0,0), n_i=(1,1,0) and n_i=(1,1,1).

n_i	k_i	h_{11}=1			h_{12}=1			h_{44}=1		
		s_{k2}	s_{n2}	s_{b2}	s_{k2}	s_{n2}	s_{b2}	s_{k2}	s_{n2}	s_{b2}
(1,0,0)	$k_i^{(1)}$	0	.500	0	0	0	0	1.500	0	0
	$k_i^{(2)}$	0	.500	0	0	0	0	1.500	0	0
	$k_i^{(3)}$	0	.500	0	0	0	0	1.500	0	0
(1,1,0)	$k_i^{(4)}$	.750	.250	0	−.750	.250	0	0	.500	0
	$k_i^{(5)}$	0	.250	0	0	.250	0	1.500	.500	0
	$k_i^{(6)}$	.375	.250	−.125	−.375	.250	.125	.750	.500	.250
(1,1,1)	$k_i^{(7)}$	.500	.167	0	−.500	.333	0	.500	.667	0
	$k_i^{(8)}$	.500	.167	0	−.500	.333	0	.500	.667	0
	$k_i^{(9)}$	.500	.167	0	−.500	.333	0	.500	.667	0

n_i=(1,0,0) and shearing directions k_i=(0,1,0), or k_i=(0,0,1), or k_i=(0,1,1), the values of s_{n1}, s_{k1}, s_{b1} are extreme values. Similarly, values for shearing plane n_i=(1,1,0) and shearing directions k_i=(1,–1,0), or k_i=(0,0,1), the values of s_{n1}, s_{k1}, s_{b1} are extreme values. For n_i=(1,1,1) there exist six equivalent shearing directions, one of them is k_i=(2,–1,–1). Next to it is situated the direction k_i=(1,–2,1). The vector k_i=(1,–1,0) bisects them. There exist six shearing directions equivalent to k_i=(1,–1,0). Because of the symmetry, the values of s_{k1}, s_{n1}, s_{b1} for n_i=(1,1,1), k_i=(2,–1,–1) or k_i=(1,–1,0) are extreme values. Table 2 gives the extreme values for copper.

3. Second order terms

For the cubic symmetry there exist six different elastic constants of the third order. In the abbreviated notation they are h_{111}, h_{112}, h_{123}, h_{144}, h_{155} and h_{456}. In the tensor notation the non-zero elastic constants are c_{111111}, c_{111122}, c_{112233}, c_{112323}, c_{113131}, c_{233112}. Other non-zero components are the result of the tensor symmetries. The elastic constants of second order contribute stress of the order ν^2. Here we calculate the stresses for the same n_i and k_i as above.

The geometrical nonlinearity is manifested in the non-zero values of s_{k2}, s_{n2} and s_{b2}. For h_{11}=1, h_{12}=1 and h_{44}=1 they are given in the Table 2.

The values of s_{k3} , s_{n3} and s_{b3} represent the material nonlinearity. For h_{111}=1, h_{112}=1 and h_{123}=1 they are given in the Table 3.

Table 4 has exactly the same structure as Table 3. It gives the values of s_{k3}, s_{n3} and s_{b3} for h_{144}=1, h_{155} =1 and h_{456} =1.

Note that the shearing plane n_i and the shearing direction k_i may be arbitrarily chosen. The vector b_i is then uniquely defined as the vector product of n_i and k_i. According to (1.16)–(1.18), the function s_{k3} is an odd function of k_i and an odd function of n_i. In contrast s_{n3} is even function of k_i and even function of n_i. And finally s_{b3} is an odd function of b_i, even function of k_i and odd function of n_i. Since b_i as the vector product is an odd function of k_i and an odd function of n_i, the function s_{b3} is an odd function of k_i, and an even function of n_i. For fixed shearing plane, a change of the shearing direction k_i into the opposite direction

$$(3.1) \qquad (k_1, k_2, k_3) \quad \Rightarrow (-k_1, -k_2, -k_3)$$

changes the signs of coefficients s_{k3} and s_{b3}, and does not change the value of s_{n3}.

With the cubic symmetry a physically more interesting, following invariance is connected. Simultaneous reflections of the vectors n_i and k_i in the (2.3), (3.1) and (1.2) coordinate planes

Table 3. Coefficients s_{k3}, s_{n3}, s_{b3} for h_{111}=1, h_{112}=1, h_{123}=1.

n_i	k_i	h_{111}=1, other $h_{\alpha\beta\gamma}$=0			h_{112}=1, other $h_{\alpha\beta\gamma}$=0			h_{123}=1, other $h_{\alpha\beta\gamma}$=0		
		s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	s_{b3}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(2)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(3)}$	0	0	0	0	0	0	0	0	0
(1,1,0)	$k_i^{(4)}$	0	.125	0	0	−.125	0	0	0	0
	$k_i^{(5)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(6)}$	0	.062	0	0	−.062	0	0	0	0
(1,1,1)	$k_i^{(7)}$	.039	.056	0	−.118	0	0	.079	−.056	0
	$k_i^{(8)}$	0	.056	−.039	0	0	.118	0	−.056	−.079
	$k_i^{(9)}$	.028	.056	−.028	−.083	0	.083	.056	−.056	−.056

Table 4. Coefficients s_{k3}, s_{n3}, s_{b3} for h_{144}=1, h_{155}=1, h_{456}=1.

n_i	k_i	h_{144}=1, other $h_{\alpha\beta\gamma}$=0			h_{155}=1, other $h_{\alpha\beta\gamma}$=0			h_{456}=1, other $h_{\alpha\beta\gamma}$=0		
		s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	S_{b3}	s_{k3}	s_{n3}	s_{b3}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	1.000	0	0	0	0
	$k_i^{(2)}$	0	0	0	0	1.000	0	0	0	0
	$k_i^{(3)}$	0	0	0	0	1.000	0	0	0	0
(1,1,0)	$k_i^{(4)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(5)}$	0	.500	0	0	.500	0	0	1.000	0
	$k_i^{(6)}$	0	.250	0	0	.250	0	0	.500	0
(1,1,1)	$k_i^{(7)}$	.236	−.333	0	−.236	.667	0	−.157	−.222	0
	$k_i^{(8)}$	0	−.333	−.236	0	.667	.236	0	−.222	.157
	$k_i^{(9)}$	.167	−.333	−.167	−.167	.667	.167	−.111	−.222	.111

$$
\begin{aligned}
&(n_1, n_2, n_3) \Rightarrow (-n_1, n_2, n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (-k_1, k_2, k_3),\\
&(n_1, n_2, n_3) \Rightarrow (n_1, -n_2, n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (k_1, -k_2, k_3),\\
&(n_1, n_2, n_3) \Rightarrow (n_1, n_2, -n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (k_1, k_2, -k_3).
\end{aligned} \tag{3.2}
$$

do not change s_{k3} and s_{n3}, and change the sign of s_{b3}. The proof based on the definitions of s_{k3}, s_{n3} and s_{b3} is elementary, but demands long calculations. It is easy to check the invariance (2.7) numerically.

4. Extreme values

In the present chapter will be analyzed the shearing planes and shearing directions for which the tractions reach extreme values. The coefficients s_{k1}, s_{n1}, s_{b1}, s_{k2}, ..., s_{b3} and their sums, e.g. $s_{k2} + s_{k3}$, will be considered separately. The independent variables are the two vectors n_i and k_i. Three constraints expressing the fact that they are unit, mutually orthogonal vectors must be taken into account. In order to avoid the constraints in computations introduce three new, real parameters $(\vartheta, \varphi, \psi)$, which enable us to write the components of the unit vectors n_i and k_i in the form

$$
\begin{aligned}
n_1 &= \sin\vartheta \cos\varphi,\\
n_2 &= \sin\vartheta \sin\varphi,\\
n_3 &= \cos\vartheta;
\end{aligned} \tag{4.1}
$$

$$
\begin{aligned}
k_1 &= \cos\psi \cos\vartheta \cos\varphi - \sin\psi \sin\varphi,\\
k_2 &= \cos\psi \cos\vartheta \sin\varphi + \sin\psi \cos\varphi,\\
k_3 &= -\cos\psi \sin y\vartheta.
\end{aligned} \tag{4.2}
$$

The two angles ϑ and φ define the vector n_i, namely its inclination to the x_3 axis and inclination of its projection on the $x_1\, x_2$ plane to the x_1 axis. These two angles define the shearing plane. The additional angle ψ, together with ϑ and φ define the shearing direction k_i, which is parallel to the shearing plane. The vector b_i is uniquely defined by the vectors n_i and k_i, as their vector product

$$
\begin{aligned}
b_1 &= -\sin\psi \cos\vartheta \cos\varphi - \cos\psi \sin\varphi,\\
b_2 &= -\sin\psi \cos\vartheta \sin\varphi + \cos\psi \cos\varphi,\\
b_3 &= \sin\psi \sin\vartheta.
\end{aligned} \tag{4.3}
$$

The triad of three mutually orthogonal unit vectors (n_i, k_i, b_i) possesses three degrees of freedom. It is uniquely defined by the three parameters ϑ, φ, ψ. For

arbitrary $(\vartheta, \varphi, \psi)$ the above three unit vectors n_i, k_i and b_i are mutually orthogonal. The functions s_k, s_n, s_b depend on n_i, k_i and b_i. If it is taken into account that b_i may be expressed by n_i and k_i, then the functions s_k, s_n, s_b depend on n_i and k_i only.

Very useful for the description of material properties is the shearing plane defined by n_i and the shearing direction k_i. From (4.1) it follows that replacement of $(\vartheta, \varphi, \psi)$ by other values results in reflection in the shearing planes and shearing directions in the coordinate planes

$$
\begin{aligned}
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (-n_1, n_2, n_3),\ (-k_1, k_2, k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, \pi - \varphi, -\psi), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, -n_2, n_3),\ (k_1, -k_2, k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, -\varphi, -\psi), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, n_2, -n_3),\ (k_1, k_2, -k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, \pi - \varphi, -\psi).
\end{aligned} \tag{4.4}
$$

Substitution of (4.1)–(4.3) into the expression for s_k given in (1.16) leads to a sum of 225 products of trigonometric functions of ϑ, φ and ψ. Due to symmetry some terms are equal zero. The same number of products appears in the expressions for s_{n3} and s_{b3} given in (1.17) and (1.18). Purely analytical approach leads to simple, but long expressions. Finding the roots would be very tedious. In practice only the numerical approach is effective.

Confine our attention to one definite material, namely to copper. Copper has the cubic symmetry of the type VIIb for which there exist only three different elastic constants of the first order h_{11}, h_{12}, h_{44} and six different elastic constants of the second order h_{111}, h_{112}, h_{123}, h_{144}, h_{155}, h_{456}, cf. [2, 3]. The elastic constants of the second and third order for copper are

$$
h_{11} = 169\,\text{GPa}, \quad h_{12} = 122\,\text{GPa}, \quad h_{44} = 73.5\,\text{GPa}, \tag{4.5}
$$

$$
\begin{aligned}
&h_{111} = -1350\,\text{GPa}, \quad h_{112} = -800\,\text{GPa}, \quad h_{123} = -120\,\text{GPa}, \\
&h_{144} = -66\,\text{GPa}, \quad h_{155} = -720\,\text{GPa}, \quad h_{456} = -32\,\text{GPa}.
\end{aligned} \tag{4.6}
$$

In cubic crystals all three principal directions are equivalent. It is easy to check that the following changes of the shearing plane (n_1, n_2, n_3) and shearing direction (k_1, k_2, k_3)

$$
\begin{aligned}
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_2, n_1, n_3),\ (k_2, k_1, k_3), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, n_3, n_2),\ (k_1, k_3, k_2), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_3, n_2, n_1),\ (k_3, k_2, k_1),
\end{aligned}
$$

do not change the properties of the crystal, i.e. the values of s_{k1}, s_{n1}, s_{b1} s_{k1},..., s_{b3}.

The above discussed symmetry properties of functions s_k, s_n, s_b allow us to confine all calculations to shearing planes defined by the vector n_i possessing non-negative components n_1, n_2 and $n_3, n_i > 0$. Such shearing planes are the most natural planes. The values for other vectors n_i, k_i follow from the symmetries of the considered problem.

Start with the values of s_{k1}, s_{n1}, s_{b1}. They express the linear part of the stress-deformation function for pure shear.

Table 5. Extreme values of s_{k1}, s_{n1}, s_{b1} for Cu.

		Value	ϑ, φ, ψ	n_i	k_i
s_{k1}	max	75.30	(.393,0,1.571)	(.383,0,.924)	(0,1,0)
	m/m	36.45	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
	min	23.50	(1.571,.785,1.571)	(.707,.707,0)	(–.707,.707,0)
s_{n1}	max	29.06	(1.261,.326,2.306)	(.902,.305,.305)	(–.431,.631,.646)
	m/m	0		(1,0,0)	(–.500,–.707,.500)
	min	–29.06	(1.263,1.245,.841)	(.305,.902,.305)	(–.638,.431,–.638)
s_{b1}	max	25.90	(–.785,3.142,.785)	(.707,0,.707)	(–.500,–.707,.500)
	m/m	0*	(1.571,0, 1.571)	(1,0,0)	(0,1,0)
	min	–25.90	(1.571,.785,.785)	(.707,.707,0)	(–.500,.500,–.707)

Maximum value is marked by "max", and minimum value by "min". An extremum, that is neither maximum, nor minimum (saddle point) is marked by "m/m". The value 0 marked by asterisk is an extremum for each ψ. For $\psi = \pi/2$ the normal to the shearing plane and the shearing direction coincide with the coordiate axes.

Pass now to the values of s_{k2}, s_{n2}, s_{b2}. They express the geometrical non-linearity of the deformation. Their values are given in Table 6. The value 84.50 marked by asterisk is an extremum for each ψ.

Table 6. Extreme values of s_{k2}, s_{n2}, s_{b2} for Cu.

		Value	ϑ, φ, ψ	n_i	k_i
s_{k2}	max	112.95	(0,.785,0)	(0,0,1)	(.707.–.707,0)
	m/m	54.68	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
	min	35.25	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
s_{n2}	max	119.03	(.955,.785,.732)	(.577,.577,.577)	(–.169,.776,–.607)
	m/m	110.40	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	min	84.50*	(0,.785,0)	(0,0,1)	(.707,.707,0)
s_{b2}	max	38.85	(.785,1.571,.785)	(0,.707,.707)	(–.707,.500,–.500)
	min	–38.85	(1.571,.785,.785)	(.707,.707,0)	(–.500,.500,–.707)

Similar calculations lead to the extreme values of s_{k3}, s_{n3}, s_{b3}. Their values are given in Table 7. Note that some of the directions in Table 6 and Table 7 do not

coincide. The extreme directions for the geometrical nonlinearity are different from that for the physical nonlinearity.

Table 7. Extreme values of s_{k3}, s_{n3}, s_{b3} for Cu.

		value	ϑ, φ, ψ	n_i	k_i
s_{k3}	max	160.59	(1.047,.615–.956)	(.707,.500,.500)	(.707.–.500,–.500)
	max	64.82	(.228,.785,0)	(.159,.159,.974)	(.689,.689,–.226)
	min	–64.82	(–.228,3.927,0)	(.150,.150,.974)	(–.689,–.689,.226)
	min	–160.59	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
s_{n3}	max	–68.75	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	max	–109.69	(.555,.785,0)	(.372,.372,.850)	(.601,.601,–.527)
	min	–360.0	(0,.785,0)	(0,0,1)	(.707,.707,0)
	min	–395.15	(1.211,.385,.715)	(.868,.352,.352)	(0,.707,–.707)
S_{b3}	max	125.24	(.887,.952,.423)	(.450,.632,.632)	(0,.707,–.707)
	max	73.75	(–.393,3.142,1.571)	(.383,0,.924)	(0,–1,0)
	min	–73.75	(.393,0,1.571)	(.383,0,.924)	(0,1,0)
	min	–125.24	(1.104,.785,1.571)	(.632,.632,.450)	(–.707,.707,0)

Since both s_{k2} and s_{k3} contribute to the stress proportionally to ν^2, important for the analysis is their sum $s_{k2} + s_{k3}$. The same holds for the sums $s_{n2} + s_{n3}$ and $s_{b2} + s_{b3}$. Table 8 gives the corresponding extreme values.

Table 8. Extreme values of $(s_{k2} + s_{k3})$, $(s_{n2} + s_{n3})$, $(s_{b2} + s_{b3})$.

		value	ϑ, φ, ψ	n_i	k_i
$s_{k2}+s_{k3}$	max	215.27	(1.047,.615–.956)	(.707,.500,.500)	(.707.–.500,–.500)
	max	167.72	(.201,.785,0)	(.141,.141,.980)	(.693,.693,–.200)
	min		(–.230,3.824,.125)	(.177,.144,.974)	(–.671,–.706,.223)
	min	35.45	(–.258,3.903,.026)	(.185,.176,.967)	(–.684,–.684,.255)
	min	–105.92	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
$s_{n2}+s_{n3}$	max	41.65	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	max	–2.05	(.569,.785,0)	(.381,.381,.841)	(.596,.596,–.538)
	max	–102.10	(1.571,.785,0)	(.707,.707,0)	(0,0,–1.000)
	min	–275.50	(0,.785,0)	(0,0,1)	(.707,.707,0)
	min	–291.9	(1.264,.323,.731)	(.904,.302,.302)	(0,.707,–.707)
$s_{b2}+s_{b3}$	max	126.35	(.861,.938,.462)	(.448,.611,.652)	(–.014,.734,–.679)
	max	75.79	(–.401,3.202,1.435)	(.024,.921,.389)	(–.996,.054,–.065)
	min	–53.2	(–.291,4.137,–.785)	(.156,.611,.448)	(–.962,–.184,.203)
	min	–75.79	(.401,1.512,1.704)	(.023,.390,.921)	(–.997,–.064,.052)
	min	–126.35	(1.060,.753,1.553)	(.652,.611,.448)	(.678,.735,–.016)

The angles (ϑ,φ,ψ) make easier the computations. Obviously, instead of the angles (ϑ,φ,ψ) the two vectors n_i, k_i may be used. Since for cubic symmetry all three directions in space are equivalent, some shearings are physically equivalent.

Note that some directions in the above tables coincide e.g. the direction (.500,.500,.707) is a common extreme direction for s_{k2} and s_{k3} (Tables 6 and 7). Such directions are in fact connected with the symmetry of the problem. Other directions, e.g. (.652,.611,.448) in the last line of Table 8 is an extreme direction for one set of elastic constants only. Such directions are specific extreme directions for one material only, namely copper.

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