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The Dissipation-Inequality of Rate-Independent Thermoplasticity

In real processes involving large plastic deformations a major part of the stress power will be dissipated and involves thermodynamical changes that cannot be neglected. A framework for the description of thermoplastic processes based on the notion of isomorphic thermoelastic ranges is suggested. Within this framework, consistent flow and hardening rules as well as necessary and sufficient conditions for the second law to hold are derived for the rate-independent case.

1. Materials with Isomorphic Elastic Ranges

We follow the usual lines to introduce the *thermokinematical process* consisting of a configuration process $\mathbf{C}(t) = \mathbf{F}(t)^T \mathbf{F}(t)$ (right CAUCHY-GREEN tensor), the temperature process $\theta(t)$, and the (material) temperature-gradient process $\mathbf{g}(t)$ as a triple forming a trajectory in the space of the independent variables, which is assumed to be continuous and piecewise continuously differentiable. Such processes form the process class of the thermomechanical material. The dependent variables $\{\mathbf{S}, \mathbf{q}, \psi, \eta\}$ are assumed to be determined by such a process, constituting the *calorodynamical state*, which consists of the material stress tensor $\mathbf{S} = \mathbf{F}^{-1}\,\mathbf{T}\,\mathbf{F}^{-T}$, the material heat flux $\mathbf{q}$, the specific HELMHOLTZ free energy ψ, and the specific entropy η. $\mathbf{F}$ denotes the deformation gradient and $\mathbf{T}$ the CAUCHY stress.

Definition. A *thermoelastic range* consists of a quintuple $\{\mathscr{E}_p, S_p, q_p, \psi_p, \eta_p\}$ with

- $\mathscr{E}_p$ being a path-connected closed subset of the space of independent variables that forms a differentiable manifold with boundary;
- a set of thermoelastic laws S_p, q_p, ψ_p, η_p being continuously differentiable on $\mathscr{E}_p$ and as such extendable onto the whole space of independent variables.

Assumption 1. (Existence of thermoelastic ranges). For any thermokinematical process $\{\mathbf{C}(t), \theta(t), \mathbf{g}(t)\}$ out of the process class there exists a thermoelastic range $\{\mathscr{E}_p, S_p, q_p, \psi_p, \eta_p\}$ such that

- its final value $\{\mathbf{C}(d), \theta(d), \mathbf{g}(d)\}$ is in $\mathscr{E}_p$, and
- for any continuation of this process that is entirely in $\mathscr{E}_p$, the calorodynamical state at its end is determined by the thermoelastic laws S_p, q_p, ψ_p, η_p through its final value

$$\begin{aligned} \mathbf{S}(t) &= S_p[\mathbf{C}(t), \theta(t), \mathbf{g}(t)] \\ \mathbf{q}(t) &= q_p[\mathbf{C}(t), \theta(t), \mathbf{g}(t)] \\ \psi(t) &= \psi_p[\mathbf{C}(t), \theta(t), \mathbf{g}(t)] \\ \eta(t) &= \eta_p[\mathbf{C}(t), \theta(t), \mathbf{g}(t)]. \end{aligned} \tag{1}$$

The basic underlying idea of the present approach is that plastic deformations do not influence the properties within the thermoelastic ranges. Mathematically this notion can be made precise by the concept of material isomorphisms.

Assumption 2. (Isomorphy of thermoelastic ranges). Let $\{\mathscr{E}_0, S_0, q_0, \psi_0, \eta_0\}$ and $\{\mathscr{E}_p, S_p, q_p, \psi_p, \eta_p\}$ be two thermoelastic ranges of the same material point. Then the thermoelastic laws are isomorphic, i. e., there exists a material isomorphism $\mathbf{P}$ such that

$$\begin{aligned} S_p(\mathbf{C}, \theta, \mathbf{g}) &= \mathbf{P}\, S_0(\mathbf{P}^T \mathbf{C}\, \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})\, \mathbf{P}^T \\ q_p(\mathbf{C}, \theta, \mathbf{g}) &= \mathbf{P}\, q_0(\mathbf{P}^T \mathbf{C}\, \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \\ \psi_p(\mathbf{C}, \theta, \mathbf{g}) &= \psi_0(\mathbf{P}^T \mathbf{C}\, \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \\ \eta_p(\mathbf{C}, \theta, \mathbf{g}) &= \eta_0(\mathbf{P}^T \mathbf{C}\, \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \end{aligned} \tag{2}$$

hold for all $\{\mathbf{C}, \theta, \mathbf{g}\}$.

$\mathbf{P}$ is an invertible tensor, which is called *plastic transformation*. For metal plasticity, $\mathbf{P}$ can be expected to be unimodular. $\mathbf{P}$ is non-symmetric for anisotropic materials. Only in the isotropic case, the rotational part of $\mathbf{P}$ is not necessary and can be ruled out by normalization [1, 6]. The practical procedure will be now to choose one thermoelastic range $\{\mathscr{E}_0, S_0, q_0, \psi_0, \eta_0\}$ as a referential one, and to transform the variables of the current one into those of the referential one, where all material functions remain unaltered even during yielding according to Assumption 1.

The boundary $\partial\mathscr{E}_p$ of some thermoelastic range is called *yield limit*. There is good reason to assume that the yield limit is independent of the temperature gradient, such that $\mathscr{E}_p$ is always the entire space in its last component. This gives rise to define a *yield criterion* $\Phi_p(\mathbf{C}, \theta)$, the kernel of which forms the yield limit

$$\Phi_p(\mathbf{C}, \theta) = 0 \quad \Leftrightarrow \quad \{\mathbf{C}, \theta\} \in \partial\mathscr{E}_p, \tag{3}$$

and its negative part the interior $\mathscr{E}_p^o$ of the thermoelastic range

$$\Phi_p(\mathbf{C}, \theta) < 0 \quad \Leftrightarrow \quad (\mathbf{C}, \theta) \in \mathscr{E}_p^o. \tag{4}$$

The *loading condition* is

$$\Phi_p(\mathbf{C}, \theta)^\bullet = tr\{\frac{\partial\Phi_p}{\partial\mathbf{C}}\,\mathbf{C}^\bullet\} + \frac{\partial\Phi_p}{\partial\theta}\,\theta^\bullet > 0. \tag{5}$$

The ansatz for the yield criterion φ that does not directly depend on the specific thermoelastic range is

$$\Phi_p(\mathbf{C}, \theta) = \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p), \tag{6}$$

which is assumed to be continuously differentiable with respect to all arguments. Here, $\mathbf{Z}_p$ is a set of internal variables primarily determining the hardening state of the material. The ansatz functions for the flow and hardening rule are suggested as

$$\mathbf{P}^\bullet\,\mathbf{P}^{-1} = p(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\bullet, \theta^\bullet) \tag{7}$$

and

$$\mathbf{Z}_p^\bullet = z(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\bullet, \theta^\bullet). \tag{8}$$

Both functions p and z contain a switcher such that $\mathbf{P}$ and $\mathbf{Z}_p$ evolve only if both conditions (3) and (5) are simultaneously fulfilled. These functions can be rate-dependent or -independent. In the present context, however, we will focus our attention to the rate-independent case. Because of this, p and z are positive homogeneous of degree one in their last arguments $\mathbf{C}^\bullet$ and $\theta^\bullet$, i. e.,

$$\mathbf{P}^\bullet\,\mathbf{P}^{-1} = \lambda\, p(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) = \lambda\,\mathbf{P}^\circ\,\mathbf{P}^{-1} \tag{9}$$

and

$$\mathbf{Z}_p^\bullet = \lambda\, z(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) = \lambda\,\mathbf{Z}_p^\circ \tag{10}$$

hold with $\lambda := |\mathbf{C}^\bullet| + |\theta^\bullet|$, $\mathbf{C}^\circ := \mathbf{C}^\bullet/\lambda$, $\mathbf{P}^\circ := \mathbf{P}^\bullet/\lambda$, $\mathbf{Z}_p^\circ := \mathbf{Z}_p^\bullet/\lambda$, and $\theta^\circ := \theta^\bullet/\lambda$.

2. The Consistency Condition

During yielding, the material must permanently fulfill the loading condition (5)

$$\Phi_p(\mathbf{C}, \theta)^\bullet = tr\{\frac{\partial\varphi}{\partial\mathbf{C}}\,\mathbf{C}^\bullet\} + \frac{\partial\varphi}{\partial\theta}\,\theta^\bullet > 0 \tag{11}$$

and remain on the current yield limit (3)

$$\Phi_p(\mathbf{C}, \theta) = \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p) = 0 \tag{12}$$

or

$$0 = \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p)^\bullet \tag{13}$$

$$= tr\{(\frac{\partial \varphi}{\partial \mathbf{P}})^T \mathbf{P}^\bullet\} + tr\{\frac{\partial \varphi}{\partial \mathbf{C}} \mathbf{C}^\bullet\} + \frac{\partial \varphi}{\partial \theta} \theta^\bullet + tr\{(\frac{\partial \varphi}{\partial \mathbf{Z}_p})^T \mathbf{Z}_p^\bullet\}$$

$$= tr\{\frac{\partial \varphi}{\partial \mathbf{C}} \mathbf{C}^\bullet\} + \frac{\partial \varphi}{\partial \theta} \theta^\bullet + tr\{(\frac{\partial \varphi}{\partial \mathbf{P}})^T \lambda \mathbf{P}^\circ\} + tr\{(\frac{\partial \varphi}{\partial \mathbf{Z}_p})^T \lambda \mathbf{Z}_p^\circ\}.$$

This equation allows to determine λ, and the *consistent flow rule* ($\otimes$: tensor product)

$$\mathbf{P}^\bullet \mathbf{P}^{-1} = p(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) (\otimes \mathbf{A}[\mathbf{C}^\bullet] + \alpha \theta^\bullet) \tag{14}$$

and the *consistent hardening rule*

$$\mathbf{Z}_p^\bullet = z(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) (\otimes \mathbf{A}[\mathbf{C}^\bullet] + \alpha \theta^\bullet) \tag{15}$$

are obtained with the tensor-valued function

$$\mathbf{A}(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) := \beta^{-1} \frac{\partial \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p)}{\partial \mathbf{C}}$$

and the scalar-valued functions

$$\alpha(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) := \beta^{-1} \frac{\partial \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p)}{\partial \theta}$$

and

$$\beta(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{Z}_p, \mathbf{C}^\circ, \theta^\circ) := tr\left[\left(\frac{\partial \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p)}{\partial \mathbf{P}}\right)^T \mathbf{P}^\circ - \left(\frac{\partial \varphi(\mathbf{P}, \mathbf{C}, \theta, \mathbf{Z}_p)}{\partial \mathbf{Z}_p}\right)^T \mathbf{Z}_p^\circ\right].$$

3. The Dissipation Inequality

The rate of the free energy is according to (2)

$$\psi_p(\mathbf{C}, \theta, \mathbf{g})^\bullet = \psi_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})^\bullet$$

$$= tr\{\frac{\partial \psi_0}{\partial \mathbf{C}} (\mathbf{P}^T \mathbf{C} \mathbf{P})^\bullet\} + \frac{\partial \psi_0}{\partial \theta} \theta^\bullet + \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot (\mathbf{P}^T \mathbf{g})^\bullet$$

$$= tr\{\mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \mathbf{C}^\bullet\} + \frac{\partial \psi_0}{\partial \theta} \theta^\bullet + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \mathbf{g}^\bullet$$

$$+ 2\, tr\{(\mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \mathbf{C} + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \otimes \mathbf{g}) \mathbf{P}^\circ \mathbf{P}^{-1} (\otimes \mathbf{A}[\mathbf{C}^\bullet] + \alpha \theta^\bullet)\}.$$

Here, all the derivatives have to be evaluated at $(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})$. The density of the stress-power is given by

$$tr\{\mathbf{T} \mathbf{F}^\bullet \mathbf{F}^{-1}\} = \tfrac{1}{2} tr\{S_p(\mathbf{C}, \theta, \mathbf{g}) \mathbf{C}^\bullet\} = \tfrac{1}{2} tr\{\mathbf{P} S_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \mathbf{P}^T \mathbf{C}^\bullet\}. \tag{16}$$

We plug this into the CLAUSIUS-DUHEM inequality

$$0 \geq -\rho^{-1} tr\{\mathbf{T} \mathbf{F}^\bullet \mathbf{F}^{-1}\} + \frac{q_p \cdot \mathbf{g}}{\rho_0 \theta} + \psi_p^\bullet + \theta^\bullet \eta_p$$

$$= -\rho^{-1} \tfrac{1}{2} tr\{\mathbf{P} S_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \mathbf{P}^T \mathbf{C}^\bullet\} + \frac{\mathbf{g} \cdot \mathbf{P} q_0}{\rho_0 \theta} + tr\{\mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \mathbf{C}^\bullet\}$$

$$+ \frac{\partial \psi_0}{\partial \theta} \theta^\bullet + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \mathbf{g}^\bullet + \theta^\bullet \eta_0$$

$$+ 2\, tr\{(\mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \mathbf{C} + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \otimes \mathbf{g}) \mathbf{P}^\circ \mathbf{P}^{-1} (\otimes \mathbf{A}[\mathbf{C}^\bullet] + \alpha \theta^\bullet)\}. \tag{17}$$

The last part is only non-zero, if both the yield (12) and the loading condition (11) are fulfilled.

Theorem.
The CLAUSIUS-DUHEM *inequality is satisfied for all thermokinematical processes, if and only if the following conditions hold*

$$S_0 = 2\rho \frac{\partial \psi_0}{\partial \mathbf{C}}, \qquad \eta_0 = -\frac{\partial \psi_0}{\partial \theta}, \qquad \frac{\partial \psi_0}{\partial \mathbf{g}} = \mathbf{o}, \qquad q_0 \cdot \mathbf{g} \le 0$$

and

$$tr(S_0\, \mathbf{C}\, p) \le 0. \tag{18}$$

Proof. The sufficiency of these conditions is obvious. We therefore consider their necessity. If the material is not in a state of yield, the last term in (17) is zero and

$$0 \ge -\rho^{-1} \tfrac{1}{2}\, tr\{\mathbf{P}\, S_0(\mathbf{P}^T \mathbf{C}\, \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})\, \mathbf{P}^T \mathbf{C}^\bullet\} + \frac{\mathbf{q}\cdot\mathbf{g}}{\rho_0 \theta} + tr\{\mathbf{P}\, \frac{\partial \psi_0}{\partial \mathbf{C}}\, \mathbf{P}^T \mathbf{C}^\bullet\} + \frac{\partial \psi_0}{\partial \theta}\, \theta^\bullet + \mathbf{P}\, \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \mathbf{g}^\bullet + \theta^\bullet \eta_0$$

remains. This can be valid for arbitrary increments $\mathbf{C}^\bullet$, $\theta^\bullet$, and $\mathbf{g}^\bullet$ only if the first four conditions hold. As the thermoelastic laws are assumed to be continuously differentiable in their entire domains, these conditions have to hold on the yield limit as well. This leads to the last condition; *q. e. d.*

These conditions essentially correspond to those of [3], although their starting point is different from ours, as it is not based on thermoelastic isomorphy. In [4] and [5], (18) appears only as a sufficient, but not as a necessary condition. This is due to additional terms in the free energy, which do not result from the isomorphy condition (see also [6]).

4. Conclusions

The present framework is a thermodynamical generalization of a purely mechanical theory [1, 2] and describes finite plastic deformations for isotropic and anisotropic materials. The objectivity of the whole theory is automatically fulfilled by the use of material variables. By the assumption of isomorphic thermoelastic ranges, the plastic transformation tensor $\mathbf{P}$ is introduced in a natural and mathematically precise way. In the context of crystal plasticity, $\mathbf{P}$ can be interpreted as the transformation of the material line elements that coincide with the lattice directions [2]. It should be noted that no constitutive decomposition nor the concept of an intermediate unloaded configuration have been used presently. By the assumed rate-independence, the flow rule and the hardening rule are given in a form consistent with the yield and loading criterion. Based on these assumptions alone, the dissipation inequality can be used to derive necessary and sufficient conditions to be imposed on the constitutive equations. The relation of the present theory to classical theories of finite plasticity based on a constitutive decomposition of the deformation into elastic and plastic parts can be found in [2]. It is shown there that the antisymmetric part of $\mathbf{P}^\bullet \mathbf{P}^{-1}$ is directly related to the *plastic spin* concept.

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