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# Finite thermoplasticity based on isomorphisms

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## Abstract

In real processes involving large plastic deformations, a major part of the stress power will be dissipated and induces thermodynamical changes that cannot be neglected in many cases. A framework for the description of elasto-plastic materials based on the notion of isomorphic thermoelastic ranges is developed. Within this framework, general forms of the 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. Within this frame, the concept of (unloaded) intermediate configurations is critically reviewed.

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## 1. Introduction

Our intention is to suggest an axiomatic framework for the description of rate-independent and rate-dependent (visco-)plastic behaviour in the presence of large deformations and large temperature changes.

One of the fundamental problems in finite plasticity theory is the definition of the internal variables and, in particular, that of some plastic or inelastic measure. Although the term ‘plastic deformation’ seems to be rather customary in engineering, it turns out in the context of large deformations that it is extremely difficult to give a precise definition for it. “There is no general agreement on how it is to be identified, either conceptually or experimentally, in the presence of finite deformations.” (Casey and Naghdi, 1992). If this is not accurately done, it leaves space for controversial interpretations.

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The concept of *unloaded states* or *intermediate configurations* in connection with a multiplicative decomposition of the deformation gradient as suggested by Eckart (1948), Lee and Liu (1967), Lee (1969), Fox (1968), and many others has some well-known shortcomings (Casey and Naghdi, 1980, 1992; Naghdi, 1990; Cleja-Tigoiu and Soós, 1990; Vidoli and Sciarra, 2002).

1. Rotations of such unloaded placements remain undetermined or arbitrary (Sidoroff, 1973; Haupt 1985, 2000).
2. The unloaded state becomes fictitious in the presence of a strong Bauschinger effect which shifts the unloaded state outside of the current elastic range. This has been experimentally observed (Ivey, 1961; Phillips et al., 1972; Phillips, 1974).
3. Problems with objectivity- and symmetry-transformations, which are somehow linked to 1. (see Green and Naghdi, 1971; Šilhavý, 1977; Dashner, 1986a).
4. Lack of a unified format to describe both isotropic and anisotropic behaviour. If we look at Khan and Huang (1995) or at Lubarda (2001), where both aspects are considered, we get the impression that such a unified theory is still not available. Some theories are limited to isotropic behaviour (see the discussion in Cleja-Tigoiu and Soós, 1990). These are in particular those which make use of a *symmetric* plastic variable like Lee (1969), Green and Naghdi (1965, 1978), Dashner (1986b), Casey and Naghdi (1992), Xiao et al. (2000), and many others, although this restriction is quite often not explicitly stated or even recognised. Other theories are made for anisotropic materials or crystal plasticity like Mandel (1972, 1973, 1974), Rice (1971), Krawietz (1986), Naghdi and Srinivasa (1994), Rubin (1994, 1996), but use concepts which become meaningless in the isotropic case.

The second defect was overcome by a suggestion of Casey and Naghdi (1992) and Casey (1998), who introduced the concept of the *state of maximal unloading* in the deformation space to define plastic deformations. However, this definition results in a symmetric plastic variable, which is not sufficient for anisotropic materials, as will be shown.

While also most of the other shortcomings can be somehow overcome, the first cannot, in principle. Rotations are important, especially for anisotropic materials. But the concept of unloading does not determine such rotations. Mandel's remedy to determine the rotations was the notion of an *isoclinic configuration*, i.e. a local reference placement with respect to which the elastic laws of all elastic ranges coincide (Mandel, 1972, 1973, 1974; the same suggestion has already been made by Teodosiu, 1970). This idea already comes quite close to the present suggestion. A similar idea stands behind the *state of relaxed strains* of Eckart (1948), the *equilibrium natural state* of Holsapple (1973), the (*local geometric*) *natural reference state* of Besseling (1968) and Besseling and v. d. Giessen (1994), the *local current relaxed configuration* of Cleja-Tigoiu (1990), the *natural configuration* by Rajagopal and Srinivasa (1998).

If we consequently follow Mandel's direction, we will arrive at the concept of *material isomorphisms* between elastic ranges. Roughly speaking, it simply states

that the elastic properties, if properly identified, are not effected by yielding. This concept is strong enough, so that the notions of unloading or of intermediate configurations or of plastic strain are not needed anymore and, thus, have been entirely removed from the present theory. Gilman (1960, p. 99) states already: “It seems very unfortunate to me that the theory of plasticity was ever cast into the mold of stress-strain relations because ‘strain’ in the plastic case has no physical meaning that is related to the material of the body in question. It is rather like trying to deduce some properties of a liquid from the shape of the container that holds it.” The notion of *elastic* or *plastic deformations* or *strains* is misleading, because none of them is related to a motion in compatible way. Such expressions provoke the impression that such plastic or elastic ‘strains’ were kinematical concepts, which is certainly false (Cleja-Tigoiu and Soós, 1990).

In contrast to this, *material isomorphy* is a very general concept in material theory, which can be applied to all mechanical/thermo/electro/magneto etc. material models (Bertram, 1982, 1989). In the context of elasto-plastic materials, we make only use of *thermoelastic* isomorphisms. And this concept applies to both isotropic and anisotropic materials in precisely the same way. Here, it constitutes a theory of *isomorphic elastic ranges* as it was worked out for the mechanical case in Bertram (1992, 1999a) (see also Šilhavý and Kratochvíl, 1977; Svendsen, 2001). It leads to the introduction of a non-symmetric second order tensor as the fundamental plastic variable, called *plastic transformation* (following Wang and Bloom, 1974; Halphen and Nguyen, 1975). Its mathematical properties can be easily determined. One of them is that it is only unique up to symmetry transformations. However, this non-uniqueness is acceptable, as it has no physically detectable influence on the resulting structure, as we will show.

These definitions bring some light into the sustaining discussion on appropriate plastic variables, as our definition is mathematically exact and leaves little space for controversial interpretations. The isomorphy of the elastic ranges is fulfilled by almost all of the competing theories of finite plasticity, although seldom stated in a clear and precise form.<sup>1</sup> But it must remain clear that it is a strong constitutive assumption, which some materials fulfil, while others do not. In Böhlke and Bertram (2001) a class of materials is investigated, for which the texture of the polycrystal has considerable influence on the elastic properties (induced elastic anisotropy). In such cases the elastic ranges are *not* isomorphic. However, the isomorphy still is a helpful concept and has been generalised there to describe such behaviour.

In Bertram (1992, 1999a) a mechanical theory for *materials with isomorphic elastic ranges* has been worked out in detail and its relation to other theories, namely those with a multiplicative or additive constitutive decomposition are given. In the presence of large plastic deformations, a major part of the mechanical power is converted into heat, which can lead to remarkable changes of temperature. The only way to properly describe this effect is to embed this framework into a complete thermodynamical setting. The elastic isomorphism becomes now a *thermoelastic*

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<sup>1</sup> As an exception, Cleja-Tigoiu and Soós (1990) do state such an assumption under the label of *temporarily invariance*. See also Lee and Germain (1974), pp. 122, 126, and Rice (1971), p. 450.

*isomorphism*, the exact form of which is known since long (see, e.g., Noll, 1958; Truesdell and Noll, 1965, sect. 27; Wang and Truesdell, 1973, p. 264; Bertram, 1989).

By substituting these constitutive expressions into the Clausius-Duhem-inequality, necessary and sufficient conditions for it can be derived.

In Bertram (1999b) this has been done, with results similar to those of Besdo (1980), Krawietz (1986), Dashner (1986b), Acharya and Shawki (1996), and many others. However, we are now convinced that this approach, although correct, is rather restrictive, as it does not account for the dissipation due to hardening. It turned out that additional constants for the energy and the entropy, which do not play an important role in thermoelasticity and are therefore usually suppressed, now in this context do become relevant. These additional parts are only constant within each thermoelastic range. If the range is changed, however, i.e., if yielding occurs, these parts can also vary. This means that they can possibly depend on all those state variables that are constant within the elastic ranges. The only variables with this property are the plastic transformation itself and the hardening variables. These parts give rise to additional dissipative terms, which remain in the residual dissipation inequality (see also the discussion in Kratochvíl and Dillon, 1970; Cleja-Tigoiu and Soós, 1990; Casey, 1998).

For real materials the assumption of rate-independence is just a coarse simplification, as measurements show creep, relaxation, and rate-dependent hysteresis for most metals even at room temperature. If one wants to include such effects in the modelling, this can easily be done by including two additional terms into the flow and hardening rule (Halphen, 1975; Halphen and Nguyen, 1975; Cleja-Tigoiu, 1990). In the Appendix it is shown that the second law renders an additional condition in form of an inequality for such models.

## 2. Thermoelastic materials

Before we introduce the concept of a thermoelastic range, we shall recall the definition of a thermoelastic material point. Furthermore, we consider the problem to identify two points exhibiting the same thermoelastic behaviour and, thus, consisting of the same material.

Before we do this, we should introduce some notations. We denote the composition of tensors of same order  $\mathbf{A}$  and  $\mathbf{B}$  by  $\mathbf{AB}$ . The application of a second-order tensor  $\mathbf{A}$  to a vector  $\mathbf{v}$  is denoted by  $\mathbf{Av}$ . The application of a fourth-order tensor  $\mathbf{C}$  to a second-order one  $\mathbf{A}$  is denoted by  $\mathbf{C}[\mathbf{A}]$ .  $\otimes$  is the tensor product. Inner products between vectors or tensors of same order are denoted by  $\cdot$ . A superscript  $T$  indicates the transposition,  $-1$  the inversion, and  $-T$  the inversion of the transposed mapping.

Let  $\mathbb{R}$  denote the reals,  $\mathbb{V}$  the Euclidean vectors,  $\text{Lin}$  the second order tensors,  $\text{Inv}$  the invertible tensors,  $\text{Orth}$  the orthogonal tensors,  $\text{Sym}$  the symmetric tensors, and  $\text{Psym}$  the positive-definite symmetric tensors. In general, a superscript  $+$  denotes the subsets of elements with positive determinant.

Let  $\mathbf{F} \in \text{Inv}^+$  be the deformation gradient and  $\mathbf{T} \in \text{Sym}$  Cauchy's stress tensor. In the present theory, the independent variables are the fields of the right Cauchy–Green

tensor  $\mathbf{C} = \mathbf{F}^T \mathbf{F} \in \text{Psym}$  and of the temperature  $\theta \in \mathbb{R}^+$ . The latter is assumed to be differentiable in space, and the material temperature-gradient is denoted by  $\mathbf{g} \in V$ . The set  $\text{Psym} \times \mathbb{R}^+ \times V$  is referred to as the (local) *thermo-kinematical state space* containing the *thermo-kinematical states*  $\{\mathbf{C}, \theta, \mathbf{g}\}$ . The dependent variables  $\{\mathbf{S}, \mathbf{q}, \epsilon, \eta\}$  consist of the 2. Piola–Kirchhoff stress tensor  $\mathbf{S} = J\mathbf{F}^{-1} \mathbf{T} \mathbf{F}^{-T} \in \text{Sym}$ , the material heat flux  $\mathbf{q} \in V$ , defined by the Eulerian heat flux  $\mathbf{q}_E$  through  $\mathbf{q} = J\mathbf{F}^{-1} \mathbf{q}_E$ , the specific internal energy  $\epsilon \in \mathbb{R}$ , and the specific entropy  $\eta \in \mathbb{R}$ . We will call this set the (local) *caloro-dynamical state*. A thermoelastic material is one, for which the thermo-kinematical state at some instant completely determines the caloro-dynamical state at the same instant. We will make this more precisely in the following definition.

**Definition.** A material point is said to be thermoelastic if it is constituted by the following four material functions for the

$$\begin{array}{ll}
 \text{stresses} & S: \\
 \text{heat flux} & q: \\
 \text{internal energy} & \epsilon: \\
 \text{entropy} & \eta:
 \end{array}
 \begin{array}{l}
 \left\{ \mathbf{C}, \theta, \mathbf{g} \right\} \mapsto \mathbf{S} \\
 \left\{ \mathbf{C}, \theta, \mathbf{g} \right\} \mapsto \mathbf{q} \\
 \left\{ \mathbf{C}, \theta, \mathbf{g} \right\} \mapsto \epsilon \\
 \left\{ \mathbf{C}, \theta, \mathbf{g} \right\} \mapsto \eta
 \end{array}
 \left| \begin{array}{l}
 \text{Psym} \times \mathbb{R}^+ \times V \rightarrow \text{Sym} \\
 \text{Psym} \times \mathbb{R}^+ \times V \rightarrow V \\
 \text{Psym} \times \mathbb{R}^+ \times V \rightarrow \mathbb{R} \\
 \text{Psym} \times \mathbb{R}^+ \times V \rightarrow \mathbb{R}
 \end{array} \right. \quad (1)$$

As we exclusively chose material or Lagrangean variables, all these variables and all these functions are invariant under changes of observer as well as under superimposed rigid body motions, and, hence, identically fulfil the Euclidean invariance principle. However, they do depend on a reference placement. This can be freely chosen, as we do not assign any specific properties to it. This opens the choice for a reference-free or intrinsic representation as suggested by Noll (1972).

The following question naturally arises. If we consider two thermoelastic material points  $X$  and  $Y$ , then what does it mean that they consist of the *same material*? The answer will be given by the following definition (see Bertram, 1999b).

**Definition.** Two thermoelastic points  $X$  and  $Y$  with material functions  $S_{X,Y}$ ,  $q_{X,Y}$ ,  $\epsilon_{X,Y}$ , and  $\eta_{X,Y}$  are isomorphic, if there exists an invertible linear mapping  $P \in \text{Inv}^+$ , called thermoelastic isomorphism, and two constants  $\epsilon_c, \eta_c \in \mathbb{R}$ , such that the following conditions hold for all thermo-kinematical states

$$\begin{aligned}
 S_Y(\mathbf{C}, \theta, \mathbf{g}) &= \det(\mathbf{P}^{-1}) \mathbf{P} S_X(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \mathbf{P}^T \\
 q_Y(\mathbf{C}, \theta, \mathbf{g}) &= \det(\mathbf{P}^{-1}) \mathbf{P} q_X(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \\
 \epsilon_Y(\mathbf{C}, \theta, \mathbf{g}) &= \epsilon_X(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \epsilon_c \\
 \eta_Y(\mathbf{C}, \theta, \mathbf{g}) &= \eta_X(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \eta_c.
 \end{aligned} \quad (2)$$

The two constants  $\epsilon_c$  and  $\eta_c$  are due to the fact, that the energy and the entropy are only determined up to some additive constants, which do not appear in any balance equation and are therefore usually suppressed in the thermoelastic context.

Isomorphy means that by the values of  $\mathbf{P}$ ,  $\epsilon_c$ , and  $\eta_c$ , the material behaviour of the two thermoelastic points is uniquely correlated. In Truesdell and Noll (1965) the following interpretation for  $\mathbf{P}$  is given.  $\mathbf{P}$  is the local change of reference-placement for  $X$  according to which the resulting constitutive equations in  $X$  and  $Y$  are identical (Wang and Truesdell, 1973, p. 264). Essentially,  $\mathbf{P}$  can be considered as an identification of

the material line elements of the two tangent spaces in  $X$  and  $Y$  to the body manifold. Once this identification is specified, the transformations for all variables are also fixed. In particular,  $\mathbf{F}$  becomes  $\mathbf{FP}$ , and the Cauchy stresses  $\mathbf{T}$  remain invariant. In most cases, and in particular for metals,  $\mathbf{P}$  will also be unimodular [ $\det(\mathbf{P}) = I$ ].

Note that the fact of whether two points are isomorphic or not does not depend on the choice of stress and strain measures. Conditions (2) can be easily transformed into equivalent ones containing other variables.

If both points are in an undistorted state, the isomorphism is a rotation and  $\mathbf{P}$  is orthogonal. Conversely, if  $\mathbf{P}$  is not orthogonal, then at least one of the two points is not in an undistorted state.

If  $X$  and  $Y$  refer to the *same* material point, then these equations are trivially fulfilled by taking the identity for  $\mathbf{P}$  and  $\varepsilon_c = \theta = \eta_c$ . In most cases, however, this is not the only choice. All such automorphisms or *symmetry transformations* constitute the *symmetry-group* of the material. More precisely, a *symmetry-transformation* for a thermoelastic point is a mapping  $\mathbf{P} \in \text{Inv}^+$ , such that Eqs. (2) hold for  $X \equiv Y$  and  $\varepsilon_c = \theta = \eta_c$  for all thermo-mechanical states. By the usual plausibility argument then, symmetry-transformations must be unimodular (Šilhavý, 1997, Chapter. 9.4).

The relations between the isomorphisms and the symmetry-transformations for a specific thermoelastic material are specified by the following theorem, which also holds in a much more general context of inelastic materials (Bertram, 1989).

### Theorem 1.

(1) (*Transformation of the symmetry group under material isomorphisms*) If  $P$  is a material isomorphism between two thermoelastic materials and  $G_0$  the symmetry group of the first, then  $G_p := P G_0 P^{-1}$  is the symmetry group of the second.

(2) (*Material isomorphisms are unique only up to both-sided symmetry transformations*) If  $P$  is a material isomorphism between two thermoelastic materials with symmetry groups  $G_0$  and  $G_p$ , respectively, then  $A_p P A_0^{-1}$  too is a material isomorphism between them for all  $A_0 \in G_0$  and  $A_p \in G_p$ .

(3) (*Material isomorphisms differ by symmetry transformations*) Let  $P$  and  $\underline{P}$  be material isomorphisms between two thermoelastic materials with symmetry groups  $G_0$  and  $G_p$ , respectively, then  $P \underline{P}^{-1} \in G_p$  and  $P^{-1} \underline{P} \in G_0$ .

By the above definitions, the proof of this theorem is straightforward and omitted for brevity (Bertram, 1992). Note, that the first part of the theorem, although quite similar and closely related, is not exactly Noll's rule (1958), the subjects of which are changes of reference placements, and not material isomorphisms between different material points.

### 3. Thermoelastic ranges

After this preparatory work limited to purely thermoelastic behaviour, we consider the general case of a material with memory. This means that the calorodynamic response does not only depend on the current thermo-kinematical state of the material point under consideration, but also on the past ones. We describe this

by a *thermo-kinematical process*, being a mapping of some closed time interval  $[0, d]$  into the thermo-kinematical state space. We assume that such a process starts at a fixed, but freely chosen initial thermo-kinematical state, and is at least continuous and piecewise continuously differentiable. Such a thermo-kinematical process is assumed to determine the caloro-dynamical state of the material point at its end (Principle of Determinism). This functional dependence can be quite different for various materials, but for thermoplastic materials it can be given a rather specific form, as we will see. For this purpose, we next define the concept of a thermoelastic range (Owen, 1968, 1970; Casey, 1998).

**Definition.** A (thermo-) elastic range consists of a quintuple  $\{E_p, S_p, q_p, \varepsilon_p, \eta_p\}$  with

- $E_p \subset \text{Psym} \times R^+ \times V$  being a path-connected closed subset of the thermo-kinematical state space that forms a differentiable manifold with boundary;
- a set of thermoelastic laws  $S_p, q_p, \varepsilon_p, \eta_p$  as in Eqs. (1) being continuously differentiable on  $E_p$ .

Usually the boundary of  $E_p$  is called *yield limit* or *yield surface*.

**Assumption 1.** (*Existence of thermoelastic ranges*). At the end of each thermo-kinematical process  $\{\mathbf{C}(t), \theta(t), \mathbf{g}(t)\}$ ,  $t \in [0, d]$ , there exists a thermoelastic range  $\{E_p, S_p, q_p, \varepsilon_p, \eta_p\}$  such that

- the terminate value of the thermo-kinematical process  $\{\mathbf{C}(d), \theta(d), \mathbf{g}(d)\}$  is in  $E_p$ ;
- for any continuation of this thermo-kinematical process that remains entirely in  $E_p$ , the caloro-dynamical state at the end of the continuation process is determined by the thermoelastic laws  $S_p, q_p, \varepsilon_p, \eta_p$  through the final value at time  $\underline{d}$

$$\begin{aligned}
 \mathbf{S} &= S_p[\mathbf{C}(\underline{d}), \theta(\underline{d}), \mathbf{g}(\underline{d})] \\
 \mathbf{q} &= q_p[\mathbf{C}(\underline{d}), \theta(\underline{d}), \mathbf{g}(\underline{d})] \\
 \varepsilon &= \varepsilon_p[\mathbf{C}(\underline{d}), \theta(\underline{d}), \mathbf{g}(\underline{d})] \\
 \eta &= \eta_p[\mathbf{C}(\underline{d}), \theta(\underline{d}), \mathbf{g}(\underline{d})].
 \end{aligned} \tag{3}$$

In other words, after each deformation process there exists such a range wherein the material behaviour is purely thermoelastic. Of course, all subsets of a thermoelastic range, which contain the final value, also constitute a thermoelastic range. We therefore will always deal with the maximal one.

Sometimes, the set  $E_p$  itself is already called thermoelastic range. In such a case we will always assume that this set is endowed with the constitutive equations  $S_p, q_p, \varepsilon_p, \eta_p$ .

As long as the continuation process remains entirely in the current elastic range, the material behaves thermoelastically. What happens, however, if the process crosses the boundary of the present elastic range. According to the above assumption, it must change the elastic range as well. Such a continuous transformation of the current elastic ranges is called *yielding*. And the primary purpose of any theory of plasticity is the description of evolving elastic ranges. This task consist of two parts, namely, firstly to model the evolution of the set  $E_p$ , or, equivalently, that of the yield surface, and secondly that of the thermoelastic laws  $S_p, q_p, \varepsilon_p, \eta_p$  associated with  $E_p$ . We start with the latter part.

For many materials, especially crystalline ones, the current elastic properties are not influenced by the past plastic yielding. For example, Young's modulus of steel or its thermal conductivity are little altered by previous forming processes (see Cleja-Tigoiu, 1990, remark on p. 173; Lee and Germain, 1974). The simplest theory for materials with elastic ranges is one, for which the thermoelastic behaviour within the different elastic ranges is assumed to remain unaltered. Roughly speaking, determine the thermoelastic constants of a sample, then perform an arbitrary deformation and temperature process, and thereafter measure the elastic constants once again. If they are the same as before, we call the initial and the final elastic ranges isomorphic. This property can be directly measured, even in a stressed and heated/cooled state. The precise formulation of this notion makes use of the introduced thermoelastic isomorphisms and gives rise to the following second assumption.

**Assumption 2.** (*Isomorphy of thermoelastic ranges*). Let  $\{E_0, S_0, q_0, \varepsilon_0, \eta_0\}$  and  $\{E_p, S_p, q_p, \varepsilon_p, \eta_p\}$  be two thermoelastic ranges of the same material point. Then the thermoelastic laws are isomorphic, i. e., there exists a material isomorphism  $\mathbf{P} \in \text{Inv}^+$  and two constants  $\varepsilon_c, \eta_c \in R$  such that

$$\begin{aligned} S_p(\mathbf{C}, \theta, \mathbf{g}) &= \det(\mathbf{P}^{-1})\mathbf{P} S_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})\mathbf{P}^T \\ q_p(\mathbf{C}, \theta, \mathbf{g}) &= \det(\mathbf{P}^{-1})\mathbf{P} q_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \\ \varepsilon_p(\mathbf{C}, \theta, \mathbf{g}) &= \varepsilon_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \varepsilon_c \\ \eta_p(\mathbf{C}, \theta, \mathbf{g}) &= \eta_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \eta_c \end{aligned} \quad (4)$$

hold for all thermo-kinematical states  $\{\mathbf{C}, \theta, \mathbf{g}\} \in \text{Psym} \times R^+ \times V$ .

Note that in this assumption nothing is said about the relation of the two sets  $E_0$  and  $E_p$ . The hardening/softening behaviour has not been restricted.

How can we identify  $\mathbf{P}$  by measurement? In principle the prescription for measuring  $\mathbf{P}$  is very simple. Identify the thermoelastic behaviour before and after yielding, and then solve Eqs. (4) for  $\mathbf{P}$ . So we reduced the measurement of a plastic variable to that of identifying thermoelasticity. Of course, in practise this is not simple at all. If the material has anisotropy axis in the elastic law like a crystal lattice, then the identification is easy.  $\mathbf{P}$  maps those material vectors in the reference configuration, which coincide with the lattice before and after yielding (Bertram, 1999, p. 367).

Physically, the conditions (4) can only be tested for values within the corresponding elastic ranges. However, we can always extend the thermoelastic functions of a

particular elastic range onto the whole thermo-kinematical state space. For example, if we choose a linear stress law, then we just use the same elasticities for all deformations, without distinguishing whether they are inside or outside of this range. By such an extension, which is entirely immaterial and has no physical consequences whatsoever, it is justified to require Eqs. (4) to hold everywhere in the space of thermo-kinematical states without need for distinguishing between the different domains of the thermoelastic functions and, thus, formally complicating the assumption.<sup>2</sup>

The practical procedure for modelling such materials becomes rather simple by these assumptions. First we choose an arbitrary, but fixed elastic range  $\{E_0, S_0, q_0, \varepsilon_0, \eta_0\}$  as an *elastic reference range*. For our purpose,  $E_0$  is not important, but only the set of thermoelastic equations. Second, we transform the current (and time dependent) constitutive functions by means of  $\mathbf{P}$  into these reference functions by Eqs. (4). We will therefore call  $\mathbf{P}$  the *plastic transformation*. In general, it cannot be interpreted as a deformation, because it cannot be derived from a motion like the deformation gradient. There is no need for defining a plastic or elastic ‘deformation’, as Rubin (1996) correctly states. Note that the elastic reference range does not involve any configuration or other kinematical notion, but just a set of thermo-mechanical equations.

The plastic transformation depends not only on the (arbitrary) choice of the reference placement, but also on the (arbitrary) choice of the elastic reference range. These two choices are conceptually independent. If the elastic reference range happens to coincide with the current one at some instant, then the identity is a possible choice for  $\mathbf{P}$  at that instant.<sup>3</sup>

If the thermoelastic laws in Eqs. (4) are isotropic, then according to Theorem 1, (1) the plastic transformation is only unique up to arbitrary rotational parts. By the polar decomposition, we can always find an orthogonal tensor such that  $\mathbf{P}$  becomes symmetric. Thus, the following theorem holds.

**Theorem 2.** If and only if the constitutive reference functions  $S_0, q_0, \varepsilon_0, \eta_0$  are isotropic, then the plastic transformation  $\mathbf{P}$  can be generally symmetrized (by normalisation).

An analogous result can be found in many papers on multiplicative decomposition. E.g., Lubliner (1980, p. 709) writes: “It is important to note that the entire tensor  $\mathbf{F}_p$ , and not merely its right Cauchy–Green Tensor  $\mathbf{C}_p = \mathbf{F}_p^T \mathbf{F}_p$ , must in general be included in a description of the state, except in certain cases of isotropy.” (Mandel, 1973 p. 726, 1982, p. 20; Anand, 1985).

<sup>2</sup> In Bertram (1992) this assumption has not been made.

<sup>3</sup> Cleja-Tigoiu and Soós (1989) p. 518 state: “... the initial value of the permanent plastic deformation (which is not an internal state variable) is in principle unknown and practically undeterminable.” This statement, which is surely correct if applied to theories based on decompositions of deformations, does not apply to the plastic transformation because of its conceptually different character. The current value of it can be experimentally determined by relating the initial thermoelastic behaviour to that of the elastic reference range.

Now we come to the other task. How can we describe the set  $E_p$  and its evolution during yielding? It turns out that this task is much more complicated than the previous one. Usually this is done by an indicator function  $\varphi$  called *yield criterion*, which assigns to each thermo-kinematical state some real number being zero on the boundary of the elastic range (yield limit), negative in its interior, and positive otherwise. As no materials are known, for which the yield limit depends on the temperature gradient, we will exclude this possibility in the sequel. In order to give the yield criterion a general form, which holds for all elastic ranges, we introduce a collection of additional internal tensorial variables and collect them in a vector  $\mathbf{H}$  out of some linear space  $\underline{\text{Lin}}$ , which has to be further specified for each particular material within this class under consideration. We will call them *hardening* (or *softening*) *variables*, although they are not restricted to this effect and may also stand for the phenomenological description of changes in the microstructure etc. The yield criterion is then a function

$$\varphi : \{\mathbf{C}, \theta, \mathbf{P}, \mathbf{H}\} \mapsto \varphi \mid \text{Psym} \times R^+ \times \text{Inv}^+ \times \underline{\text{Lin}} \rightarrow R$$

such that

$$\varphi(\mathbf{C}, \theta, \mathbf{P}, \mathbf{H}) \left\{ \begin{array}{l} < 0 \text{ in the interior} \\ = 0 \text{ on the boundary} \\ > 0 \text{ outside} \end{array} \right\} \text{ of the current elastic range.}$$

For the sake of simplicity, we will further on assume that this function is differentiable with respect to all its arguments, being aware of problems that arise with corner theories. Note that we introduce the yield criterion in the thermo-kinematical state space, which does not contain the stresses. In this we follow Besdo (1980, 1981), Casey and Naghdi (1981), Lubliner (1986), Srinivasa (1997), Wang and Barkey (1998), and others.

By means of the elastic laws we can transform it into the calorodynamical state space, if this is preferred (Dashner, 1986b, sect. 4).

Yielding will occur if and only if the thermo-kinematical process does not only hit the current yield limit, but also penetrates it, i.e., only if both

$$\bullet \text{ the yield condition } \varphi(\mathbf{C}, \theta, \mathbf{P}, \mathbf{H}) = 0 \quad (5)$$

$$\bullet \text{ the loading condition } \kappa := \frac{\partial \varphi}{\partial \mathbf{C}} \cdot \mathbf{C}^* + \frac{\partial \varphi}{\partial \theta} \cdot \theta^* > 0 \quad (6)$$

are simultaneously fulfilled. The superimposed dot denotes the (material) time derivative. The scalar  $\kappa$  is not a complete differential of  $\varphi$ , as the plastic and hardening variables are held fixed. We call  $\kappa$  the *loading parameter* (Lubliner, 1973). We must admit that the expression “loading” could be misleading, as an increase of loads or stresses is not necessarily implied when Eq. (6) holds. As the yield criterion is defined on the thermo-kinematical state space, such a “loading” can either be accompanied by a positive stress-increment (hardening) or by a negative one (softening).

For many materials the yield limit also depends on the temperature. Mostly the limit decreases, if the temperature increases, but there are also counterexamples like

the superalloys, where it is just reverse. Thus, “loading” can also mean a change of temperature, even cooling.

If both conditions (5) and (6) hold, the elastic range will necessarily be changed, and we are now able to express its change by the evolution of only two finite dimensional variables, namely  $\mathbf{P}$  and  $\mathbf{H}$ . We assume that this is governed by two evolution equations of the following form

- the flow rule  $\mathbf{P}^\bullet = p(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\bullet, \theta^\bullet)$
- the hardening rule  $\mathbf{H}^\bullet = h(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\bullet, \theta^\bullet)$

with the functions

$$p : \text{Inv}^+ \times \text{Psym} \times R^+ \times V \times \underline{\text{Lin}} \times \text{Lin} \times R \rightarrow \text{Lin}$$

$$h : \text{Inv}^+ \times \text{Psym} \times R^+ \times V \times \underline{\text{Lin}} \times \text{Lin} \times R \rightarrow \underline{\text{Lin}}$$

which contain a switcher such that  $\mathbf{P}$  and  $\mathbf{H}$  evolve only if both conditions (5) and (6) 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. (The rate-dependent case is considered in the [Appendix](#).) In this case, both rules must be positive homogeneous of first degree in  $\mathbf{C}^\bullet$  and  $\theta^\bullet$ . This can be achieved in the usual way by determining only the direction of the plastic flow and the hardening through constitutive equations, while the magnitude of both depends on a *plastic consistency parameter*  $\lambda$ . For that purpose, we introduce the following useful notation for the direction of the flow rate

$$\mathbf{P}^\circ = p^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) = \mathbf{P}^\bullet / \lambda \tag{7}$$

and of the hardening rate

$$\mathbf{H}^\circ = h^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) = \mathbf{H}^\bullet / \lambda \tag{8}$$

where  $\mathbf{C}^\circ$  and  $\theta^\circ$  denote the (arbitrarily) normalised rates of  $\mathbf{C}$  and  $\theta$ , and  $p^\circ$  and  $h^\circ$  the restrictions of  $p$  and  $h$ , respectively, to such normalised rates. The author does not see any advantage in decomposing any of these rates into symmetric and skew parts. From crystal plasticity, e.g., we know that both parts of the flow rule can be naturally given by one single evolution equation ([Bertram, 1999a](#)).

The plastic consistency parameter  $\lambda$  can be determined by the *consistency condition*, which assures that the state remains on the yield surface during yielding

$$\begin{aligned} 0 &= \varphi(\mathbf{C}, \theta, \mathbf{P}, \mathbf{H})^\bullet \\ &= \frac{\partial \varphi}{\partial \mathbf{C}} \cdot \mathbf{C}^\bullet + \frac{\partial \varphi}{\partial \theta} \cdot \theta^\bullet + \frac{\partial \varphi}{\partial \mathbf{P}} \cdot \mathbf{P}^\bullet + \frac{\partial \varphi}{\partial \mathbf{H}} \cdot \mathbf{H}^\bullet \\ &= \frac{\partial \varphi}{\partial \mathbf{C}} \cdot \mathbf{C}^\bullet + \frac{\partial \varphi}{\partial \mathbf{P}} \cdot \lambda \mathbf{P}^\circ + \frac{\partial \varphi}{\partial \mathbf{H}} \cdot \lambda \mathbf{H}^\circ \\ &= \kappa - \lambda \alpha \quad \text{with } \alpha := -\frac{\partial \varphi}{\partial \mathbf{P}} \cdot \mathbf{P}^\circ - \frac{\partial \varphi}{\partial \mathbf{H}} \cdot \mathbf{H}^\circ. \end{aligned}$$

The solution for  $\lambda$  is always positive during yielding and zero otherwise, i.e., the Kuhn–Tucker conditions always hold:  $\lambda \geq 0$ ,  $\dot{\varphi} \leq 0$ ,  $\lambda \dot{\varphi} = 0$ . By substituting  $\lambda$  into Eqs. (7) and (8), we obtain the *consistent flow* and *hardening rule*

$$\mathbf{P}^\bullet = \kappa/\alpha \mathbf{P}^\circ \tag{10}$$

$$\mathbf{H}^\bullet = \kappa/\alpha \mathbf{H}^\circ \tag{11}$$

respectively, both being functions of  $(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\bullet, \theta^\bullet)$ . Consistent means that these rules identically fulfil the consistency condition, whatever one may choose for the functions  $\varphi$ ,  $p^\circ$ , and  $h^\circ$ . We can also bring them into a form, which contains two switchers and automatically obeys the conditions (5) and (6) by means of the Macaulay brackets  $\langle \cdot \rangle$  and the Heaviside function  $H$  (Mandel, 1973, p. 734; Xiao et al., 2000, p. 158), which equals zero for negative arguments and 1 otherwise

$$\mathbf{P}^\bullet = \langle \kappa \rangle H(\varphi) / \alpha \mathbf{P}^\circ$$

$$\mathbf{H}^\bullet = \langle \kappa \rangle H(\varphi) / \alpha \mathbf{H}^\circ.$$

#### 4. The dissipation inequality

We will next investigate the restrictions of the second law on the present material class. The two additive parts  $\varepsilon_c$  and  $\eta_c$  in the isomorphy conditions for the internal energy and the entropy, respectively, are only constant within the specific elastic range. If the latter is changed, however, these parts can vary as well. It is only consequent to assume that they depend on all inelastic internal variables (Kröner and Teodosiu, 1972, p. 69), namely  $\mathbf{P}$  and  $\mathbf{H}$

$$\begin{array}{l|l} \varepsilon_c = \varepsilon_c(\mathbf{P}, \mathbf{H}) & \varepsilon_c : \text{Inv}^+ \times \underline{\text{Lin}} \rightarrow \mathbf{R} \\ \eta_c = \eta_c(\mathbf{P}, \mathbf{H}) & \eta_c : \text{Inv}^+ \times \underline{\text{Lin}} \rightarrow \mathbf{R}. \end{array} \tag{13}$$

It is convenient to introduce the specific *Helmholtz free energy*  $\psi := \varepsilon - \theta \eta \in \mathbf{R}$ , for which the isomorphy condition results in the form

$$\psi_p(\mathbf{C}, \theta, \mathbf{g}) = \psi_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \psi_c(\mathbf{P}, \mathbf{H}) - \theta \eta_c(\mathbf{P}, \mathbf{H}) \tag{14}$$

with

$$\psi_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) := \varepsilon_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) - \theta \eta_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})$$

and the additional part

$$\psi_c(\mathbf{P}, \mathbf{H}) := \varepsilon_c(\mathbf{P}, \mathbf{H}).$$

An additive decomposition of the free energy is quite often postulated (Mandel, 1974; Halphen and Nguyen, 1975; Anand, 1985; Dogui and Sidoroff, 1985; Lubliner, 1986; Svendsen, 1998). In our case it is a consequence of Assumption 2. In contrast to the form of Eq. (14), some authors, like Teodosiu (1997) assume a general temperature dependence of these additional parts. This, however, contradicts our Assumption 2 and cannot be described in this format.

The rate of the free energy according to Eq. (14) and Eqs. (4), (7), and (8) is

$$\begin{aligned} \dot{\psi} &= \dot{\psi}_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \dot{\psi}_c(\mathbf{P}, \mathbf{H}) - \dot{\theta} \eta_c(\mathbf{P}, \mathbf{H}) - \theta \dot{\eta}_c(\mathbf{P}, \mathbf{H}) \\ &= \frac{\partial \psi_0}{\partial \mathbf{C}} \cdot (\mathbf{P}^T \mathbf{C} \mathbf{P}) + \frac{\partial \psi_0}{\partial \theta} \cdot \dot{\theta} + \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot (\mathbf{P}^T \mathbf{g}) + \frac{\partial \psi_c}{\partial \mathbf{P}} \cdot \dot{\mathbf{P}} + \frac{\partial \psi_c}{\partial \mathbf{H}} \cdot \dot{\mathbf{H}} - \dot{\theta} \eta_c(\mathbf{P}, \mathbf{H}) \\ &\quad - \theta \left( \frac{\partial \eta_c}{\partial \mathbf{P}} \cdot \dot{\mathbf{P}} + \frac{\partial \eta_c}{\partial \mathbf{H}} \cdot \dot{\mathbf{H}} \right) \\ &= \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \cdot \dot{\mathbf{C}} + \frac{\partial \psi_0}{\partial \theta} \cdot \dot{\theta} + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \dot{\mathbf{g}} - \dot{\theta} \eta_c(\mathbf{P}, \mathbf{H}) \\ &\quad + \left( 2 \mathbf{C} \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} + \mathbf{g} \otimes \frac{\partial \psi_0}{\partial \mathbf{g}} + \frac{\partial \psi_c}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c}{\partial \mathbf{P}} \right) \cdot \lambda \mathbf{P}^\circ + \left( \frac{\partial \psi_c}{\partial \mathbf{H}} - \theta \frac{\partial \eta_c}{\partial \mathbf{H}} \right) \cdot \lambda \mathbf{H}^\circ. \end{aligned} \tag{15}$$

Here,  $\frac{\partial \psi_0}{\partial \mathbf{C}}$  means the partial derivative with respect to the first argument evaluated at  $(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})$ , and the other partial derivatives have an analogous meaning. All partial derivatives with respect to symmetric tensors are also taken as symmetric.

The specific stress-power is given by

$$\begin{aligned} p &:= \rho^{-1} \mathbf{T} \cdot \mathbf{F} \mathbf{F}^{-1} = 1/2 \rho_0^{-1} \mathbf{S} \cdot \dot{\mathbf{C}} = 1/2 \rho_0^{-1} S_p(\mathbf{C}, \theta, \mathbf{g}) \cdot \dot{\mathbf{C}} \\ &= 1/2 \rho_0^{-1} \det(\mathbf{P}^{-1}) \mathbf{P} S_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \mathbf{P}^T \cdot \dot{\mathbf{C}}. \end{aligned} \tag{16}$$

We substitute Eqs. (4), (7), (8), (15) and (16) into the Clausius–Duhem inequality

$$\begin{aligned} 0 &\geq -p + \frac{\mathbf{q} \cdot \mathbf{g}}{\rho_0 \theta} + \dot{\psi} + \eta \dot{\theta} \\ &= -1/2 \rho_0^{-1} S_p(\mathbf{C}, \theta, \mathbf{g}) \cdot \dot{\mathbf{C}} + q_p(\mathbf{C}, \theta, \mathbf{g}) \cdot \frac{\mathbf{g}}{\rho_0 \theta} + \dot{\psi}_p(\mathbf{C}, \theta, \mathbf{g}) \\ &\quad + \eta_p(\mathbf{C}, \theta, \mathbf{g}) \dot{\theta} \\ &= -1/2 \rho_0^{-1} \det(\mathbf{P}^{-1}) \mathbf{P} S_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \mathbf{P}^T \cdot \dot{\mathbf{C}} + \frac{\mathbf{g}}{\rho_0 \theta} \cdot \det(\mathbf{P}^{-1}) \\ &\quad \mathbf{P} q_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \cdot \dot{\mathbf{C}} + \frac{\partial \psi_0}{\partial \theta} \cdot \dot{\theta} + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \dot{\mathbf{g}} \\ &\quad + \eta_0(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g}) \dot{\theta} + \left( 2 \mathbf{C} \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} + \mathbf{g} \otimes \frac{\partial \psi_0}{\partial \mathbf{g}} + \frac{\partial \psi_c}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c}{\partial \mathbf{P}} \right) \\ &\quad \cdot \lambda \mathbf{P}^\circ + \left( \frac{\partial \psi_c}{\partial \mathbf{H}} - \theta \frac{\partial \eta_c}{\partial \mathbf{H}} \right) \cdot \lambda \mathbf{H}^\circ. \end{aligned} \tag{17}$$

The last two parts are only non-zero, if both the yield condition (5) and the loading condition (6) are fulfilled.

**Theorem 3.** *The Clausius–Duhem inequality is satisfied for all thermo-kinematical processes, if and only if the following conditions hold:*

- (1) *the free energy does not depend on the temperature gradient;*
- (2) *the Gibbs relations for the stresses*

$$S_0 = 2 \rho_0 \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \quad (18)$$

and for the entropy

$$\eta_0 = -\frac{\partial \psi_0}{\partial \theta}; \quad (19)$$

- (3) *the heat-conduction inequality*

$$\mathbf{q} \cdot \mathbf{g} \leq 0; \quad (20)$$

- (4) *and during yielding the residual inequality*

$$\begin{aligned} \mathbf{S}^p \cdot \mathbf{P}^* - \left( \frac{\partial \psi_c(\mathbf{P}, \mathbf{H})}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c(\mathbf{P}, \mathbf{H})}{\partial \mathbf{P}} \right) \cdot \mathbf{P}^* \\ - \left( \frac{\partial \psi_c(\mathbf{P}, \mathbf{H})}{\partial \mathbf{H}} - \theta \frac{\partial \eta_c(\mathbf{P}, \mathbf{H})}{\partial \mathbf{H}} \right) \cdot \mathbf{H}^* \geq 0 \end{aligned} \quad (21)$$

with  $\mathbf{S}^p := -\rho_0^{-1} \mathbf{C} \mathbf{S} \mathbf{P}^{-T} \in \text{Lin}$ .

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

$$\begin{aligned} 0 \geq 1/2 \rho_0^{-1} \det(\mathbf{P}^{-1}) \mathbf{P} S_0 \mathbf{P}^T \cdot \mathbf{C}^* + \frac{q_0 \cdot \mathbf{g}}{\rho_0 \theta} + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} \mathbf{P}^T \cdot \mathbf{C}^* + \frac{\partial \psi_0}{\partial \theta} \cdot \theta^* + \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{g}} \cdot \mathbf{g}^* \\ + \eta_0 \theta^* \end{aligned}$$

remain, where all functions depend on  $(\mathbf{P}^T \mathbf{C} \mathbf{P}, \theta, \mathbf{P}^T \mathbf{g})$ . This can be valid for arbitrary increments  $\mathbf{C}^*$ ,  $\theta^*$ , and  $\mathbf{g}^*$  if and 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 residual inequality; q.e.d.

In most cases, the first term in (21) will be positive during yielding. However, in the presence of a strong Bauschinger effect, it may eventually also become negative. In such cases, the other two terms will give the corrections for the inequality to remain permanently valid. These terms have been motivated by Sidoroff (1975), Teodosiu and Sidoroff (1976), Dogui and Sidoroff (1985), and Anand (1985).<sup>4</sup>

<sup>4</sup> See also the discussion of Rubin (1994, p. 2628) and Svendsen (1998).

Considering the heat-conduction inequality (20), we know from the isomorphy condition (4.2), that all  $q_p$  belonging to different elastic ranges, automatically fulfil it, if and only if  $q_0$  does.

By Eqs. (7), (8), and (18), the residual inequality (21) can be given the equivalent form

$$\left( 2 \mathbf{C} \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} + \frac{\partial \psi_c}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c}{\partial \mathbf{P}} \right) \cdot p^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) + \left( \frac{\partial \psi_c}{\partial \mathbf{H}} - \theta \frac{\partial \eta_c}{\partial \mathbf{H}} \right) \cdot h^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) \leq 0.$$

For given thermoelastic laws, this inequality restricts the rules for the directions of flow [Eq. (7)] and hardening [Eq. (8)], the consequences of which are beyond the scope of this paper.

The complete format for such thermoelasto-plastic materials is constituted by

- the free energies  $\psi_0(\mathbf{C}, \theta)$  and  $\psi_c(\mathbf{P}, \mathbf{H}) - \theta \eta_c(\mathbf{P}, \mathbf{H})$
- the referential law for the heat flux  $q_0(\mathbf{C}, \theta, \mathbf{g})$ .
- the yield criterion  $\varphi(\mathbf{C}, \theta, \mathbf{P}, \mathbf{H})$
- the rule for the flow direction  $p^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ)$
- the rule for the hardening direction  $h^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ)$

### 5. Intermediate configurations

If we eliminate in the above format the temperature from the list of variables, we obtain an isothermal model, which describes the purely mechanical behaviour. This leads to the following concept, where, by an abuse of notation, we use the same symbols for the restricted functions as before.

An *elastic range* consists of  $\{E_p, S_p\}$  with

- $E_p$  being a path-connected closed subset of the kinematic state space  $\text{Psym}$  that forms a differentiable manifold with boundary;
- an elastic law  $S_p$  being continuously differentiable on  $\text{Psym}$ .

At the end of each deformation process  $\{\mathbf{C}(t), t \in [0, d]\}$ , the existence of an elastic range  $\{E_p, S_p\}$  is assumed such that its final value  $\{\mathbf{C}(d)\}$  is in  $E_p$ , and for any continuation of this process that remains entirely in  $E_p$ , the stress state at its end is determined by the elastic law  $S_p$  through its final value at time  $d$

$$\mathbf{S} = S_p(\mathbf{C}(\underline{d})). \tag{22}$$

The yield criterion can be introduced in the strain space with additional hardening variables  $\mathbf{H}$  as

$$\varphi(\mathbf{C}, \mathbf{P}, \mathbf{H}). \quad (23)$$

Yielding will occur if and only if the two conditions are simultaneously fulfilled

- the yield condition  $\varphi(\mathbf{C}, \mathbf{P}, \mathbf{H}) = 0$  (24)

- the loading condition  $\kappa = \frac{\partial \varphi}{\partial \mathbf{C}} \cdot \mathbf{C}^\bullet > 0.$  (25)

For the plastic transformation and for the hardening variables we assume evolution equations

$$\mathbf{P}^\bullet = p(\mathbf{P}, \mathbf{C}, \mathbf{H}, \mathbf{C}^\bullet) \quad (26)$$

$$\mathbf{H}^\bullet = h(\mathbf{P}, \mathbf{C}, \mathbf{H}, \mathbf{C}^\bullet) \quad (27)$$

and, more specifically for the rate-independent case, by two functions giving the directions of  $\mathbf{P}$  and  $\mathbf{H}$

$$\mathbf{P}^\circ := \mathbf{P}^\bullet / \lambda = p^\circ(\mathbf{P}, \mathbf{C}, \mathbf{H}, \mathbf{C}^\circ) \quad (28)$$

$$\mathbf{H}^\circ := \mathbf{H}^\bullet / \lambda = h^\circ(\mathbf{P}, \mathbf{C}, \mathbf{H}, \mathbf{C}^\circ) \quad (29)$$

An example for such rules is given by a *plastic potential* in the form

$$\pi(\mathbf{S}^p, \mathbf{S}^h) \quad | \quad \pi : \text{Lin} \times \underline{\text{Lin}} \rightarrow R$$

with some back-stress  $\mathbf{S}^h \in \underline{\text{Lin}}$  being conjugate to  $\mathbf{H} \in \underline{\text{Lin}}$ . Then

$$\mathbf{P}^\bullet = \lambda \frac{\partial \pi(\mathbf{S}^p, \mathbf{S}^h)}{\partial \mathbf{S}^p}$$

$$\mathbf{H}^\bullet = \lambda \frac{\partial \pi(\mathbf{S}^p, \mathbf{S}^h)}{\partial \mathbf{S}^h}.$$

If we express  $\mathbf{S}^p$  through the configuration by Eq. (2), we obtain a special example of (23). However, we will not assume the existence of such a potential in the sequel, because this seems to be too restrictive.

The consistency condition assures that the state remains on the current yield surface during yielding

$$\begin{aligned} \varphi(\mathbf{C}, \mathbf{P}, \mathbf{H})^\bullet &= 0 \\ &= \frac{\partial \varphi}{\partial \mathbf{C}} \cdot \mathbf{C}^\bullet + \frac{\partial \varphi}{\partial \mathbf{P}} \cdot \mathbf{P}^\bullet + \frac{\partial \varphi}{\partial \mathbf{H}} \cdot \mathbf{H}^\bullet = \kappa + \lambda \left( \frac{\partial \varphi}{\partial \mathbf{P}} \cdot \mathbf{P}^\circ + \frac{\partial \varphi}{\partial \mathbf{H}} \cdot \mathbf{H}^\circ \right) \end{aligned} \quad (30)$$

and the *consistent flow* and *hardening rules* are

$$\mathbf{P}^\bullet = \langle \kappa \rangle H(\varphi) / \alpha \mathbf{P}^\circ \quad (31)$$

$$\mathbf{H}^* = \langle \kappa \rangle H(\varphi) / \alpha \mathbf{H}^\circ. \tag{32}$$

This completes the mechanical format for the isothermal case.

In many theories on finite plasticity the notion of intermediate unloaded configurations plays a key role. In order to relate such theories to the present one, we consider the following

**Problem.** For a material point with isomorphic elastic ranges the following shall be known.

- the elastic reference law  $S_0$
- the current unloaded configuration  $C_p$

Then, is the current elastic law  $S_p$  determined?

For the unloaded configuration most authors use an unloaded placement  $F_p$ . Clearly, by the usual invariance requirements, such an unloaded state is only determined up to arbitrary rotations. Precisely these rotations are ruled out by using

$$C_p = F_p^T F_p = F_p^T Q^T Q F_p \quad \forall Q \in \text{Orth.}$$

By the isomorphy condition (4.1) we know that the current unloaded configuration  $C_p$  is related to the unloaded configuration  $C_0$  for the elastic reference law  $S_0$  by

$$C_p = P^T C_0 P. \tag{33}$$

The current elastic law is determined according to Eq. (4.1), if we know the plastic transformation  $P$ . Thus, our problem is equivalent to solving this Eq. (33) for given  $C_p, C_0 \in \text{Psym}$ .

This equation has as many solutions as there are orthogonal tensors in Orth. This can easily be seen, if we chose the reference placement stress free for the elastic reference law. In this case,  $C_0$  is the identity tensor. Then  $P = R C_p^{1/2}$  solves Eq. (33) for all  $R \in \text{Orth}$ .

Thus, we have shown that, in general, the unloaded configuration is not sufficient to determine the current elastic law  $S_p$  for an elastoplastic material, even if we assume the validity of the isomorphy condition. However, if the elastic law is isotropic, then according to [Theorem 2](#) the plastic transformation is unique only up to arbitrary rotational parts, and the knowledge of the unloaded configuration contains sufficient information to solve the above Problem. For the anisotropic case an additional assumption is needed then. And the existence of an (isoclinic) placement, with respect to which the elastic laws of all elastic ranges are identical, is such an additional assumption, which comes close to our Assumption 2. The notion of unloading, however, is then unnecessary and can be dropped, same as a constitutive decomposition of the deformation into elastic and plastic parts anyhow.

## 6. Conclusions

In every plasticity theory, two fundamental problems have to be primarily solved, namely the introduction of a plastic variable, and of hardening variables. In the present work, we have at least solved the first of these problems in a rational way, while the second remains for further suggestions. The plastic transformation  $\mathbf{P}$  is based on a mathematically precise definition and has a clear physical interpretation (which is not that of a partial deformation). We know about its properties, in particular that it is an invertible tensor, and only unique up to both-sided symmetry transformations of the elastic law. As a consequence, it is non-symmetric in general, but can be symmetrized for isotropic materials. The non-uniqueness, however, is physically undetectable and, hence, irrelevant.

If the initial elastic range is taken as the reference one, a natural initial value of  $\mathbf{P}$  is the identity. Starting from this value, one has to integrate the flow and hardening rule for the given thermo-kinematical process, and thus obtains the accompanying process of the internal variables  $\mathbf{P}$  and  $\mathbf{H}$ . If the symmetry group is discrete, as it is the case for crystals, the evolution of  $\mathbf{P}$ , if it is continuous, rules out the ambiguity of it.

The present format describes a broad class of rate-independent materials undergoing large plastic deformations and temperature changes. It is motivated by micro-physical understanding of plastic deformations as they occur in crystals. Here the stresses depend on the deformation of the lattice, which sustains even under very large inelastic deformations. The latter are mainly due to dislocation movements, which do not alter the lattice. This leads to the concept of isomorphic elastic ranges, which also implies that the elastic constants remain the same (material isomorphy).

It should be noted here that also for the theories of Besseling (1966), Lee and Liu (1967), Lee (1969), Fox (1968), Rice (1971), Mandel (1972, 1973, 1974), Lee and Germain (1974), Halphen (1975), Anand (1985), Dashner (1986b), Cleja-Tigoiu and Soos (1990), Hackl (1997), Xiao et al. (2000), and many others the isomorphy condition essentially holds, in contrast to Krawietz (1981, 1986), who suggested a more general concept.

We have posed these concepts into thermodynamics using the Clausius-Duhem-inequality as a restriction of the material behaviour, which is standard in material modelling, although not without contradiction (Šilhavý, 1997, Chpt. 9.5). We are not saying that this is the only possible way to do this. However, it gives necessary and sufficient conditions, which are not unexpected. Firstly, we obtain the usual Gibbs potentials and the heat conduction inequality as known from thermoelasticity. Secondly, a residual inequality remains, which contains the dissipation due to both yielding and hardening. The assumption of isomorphic thermoelastic ranges implies that inelastic processes additionally contribute to both the entropy and the energy.

In Bertram (1999a) these concepts are related to those of the well-known additive and multiplicative decompositions. In contrast to them, the present approach has the following properties.

- We did not use a decomposition of the total deformation into elastic and plastic parts. The notion of ‘plastic deformation’ is not even introduced (Eckart, 1948; Gilman, 1960; Besseling, 1966; Rubin, 1994, 1996, 2001).
- We do not make use of a conceptual unloading or relaxing. On the contrary, the elastic ranges are not assumed to necessarily contain a stress-free state.
- The reference placement can be arbitrarily chosen. No special properties are assigned to it.
- Objectivity has been identically fulfilled by the use of reduced forms in the sense of Noll (1958) or, more general, of Bertram and Svendsen (2001). All variables used in the material models are material ones,<sup>5</sup> which means invariance under Euclidean transformations. If one, however, prefers objective (spatial, Eulerian) variables, all our variables can easily be transformed into the Euclidean space and the resulting format renders objective.
- No part of the deformations is assumed to be small. In fact, if the elastic range covers the whole thermo-kinematical space, the theory degenerates into an invariant and general form of finite thermoelasticity.<sup>6</sup>

In the present context, we restricted ourselves to the rate-independent case. This format can be easily generalised to also include rate-dependence (viscoplasticity) as shown in the Appendix. Applications and specifications of this format within crystal plasticity can be found in Bertram and Kraska (1995a,b).

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### Appendix. Viscoplastic extension

In order to include rate-effects like creep, relaxation, rate-dependent hysteresis, etc., we add a rate-dependent relaxation term to the flow and hardening rule

$$\begin{aligned} \mathbf{P}^* &= \lambda p^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) + r(\mathbf{P}, \mathbf{C}, \theta, \mathbf{H}) \\ \mathbf{H}^* &= \lambda h^\circ(\mathbf{P}, \mathbf{C}, \theta, \mathbf{g}, \mathbf{H}, \mathbf{C}^\circ, \theta^\circ) + s(\mathbf{P}, \mathbf{C}, \theta, \mathbf{H}) \end{aligned} \quad (34)$$

with two functions of the state variables

<sup>5</sup> In this we follow Lubliner (1973) and Krawietz (1986).

<sup>6</sup> In Lee and Germain (1974) situations are described, where both the elastic and the plastic ‘strains’ are of equal finite order.

$$\begin{array}{l|l}
 r : \{\mathbf{P}, \mathbf{C}, \theta, \mathbf{H}\} \mapsto \mathbf{P}_r^* & \text{Inv}^+ \times \text{Psym} \times R^+ \times \underline{\text{Lin}} \rightarrow \text{Lin} \\
 s : \{\mathbf{P}, \mathbf{C}, \theta, \mathbf{H}\} \mapsto \mathbf{H}_r^* & \text{Inv}^+ \times \text{Psym} \times R^+ \times \underline{\text{Lin}} \rightarrow \underline{\text{Lin}}
 \end{array}$$

while the other constitutive functions Eqs. (1)–(5) are assumed to remain valid in the same form as in the rate-independent case. If  $r$  gives a non-zero value for some state, then a change of the dependent variables takes place, even for constant deformation and temperature. This is the relaxation property. If we transform the deformation into a stress by means of the elastic law, then possibly a change of the dependent variables can take place for states of constant stresses. Thus the ansatz also describes creep.

The consistency condition during yielding is now

$$0 = \kappa - \lambda\alpha + \frac{\partial\varphi}{\partial\mathbf{P}} \cdot \mathbf{P}_r^* + \frac{\partial\varphi}{\partial\mathbf{H}} \cdot \mathbf{H}_r^*. \tag{35}$$

If the state is below the yield limit or if the loading condition is not fulfilled, then still  $\lambda=0$ . However, the material does not behave thermoelastically anymore in the absence of yielding, but may also change the ‘elastic ranges’ due to the additional terms. And also during yielding, these terms may remain active. We obtain the consistent flow and hardening rules then

$$\begin{aligned}
 \mathbf{P}^\bullet &= \frac{\left( \kappa + \frac{\partial\varphi}{\partial\mathbf{P}} \cdot \mathbf{P}_r^* + \frac{\partial\varphi}{\partial\mathbf{H}} \cdot \mathbf{H}_r^* \right)}{\alpha} \mathbf{P}^\circ + \mathbf{P}_r^* \\
 \mathbf{H}^\bullet &= \frac{\left( \kappa + \frac{\partial\varphi}{\partial\mathbf{P}} \cdot \mathbf{P}_r^* + \frac{\partial\varphi}{\partial\mathbf{H}} \cdot \mathbf{H}_r^* \right)}{\alpha} \mathbf{H}^\circ + \mathbf{H}_r^*,
 \end{aligned} \tag{36}$$

If we substitute this into the Clausius–Duhem-inequality, we obtain

$$\begin{aligned}
 0 \geq & -1/2\rho_0^{-1}\det(\mathbf{P}^{-1})\mathbf{P}S_0(\mathbf{P}^T\mathbf{C}\mathbf{P}, \theta, \mathbf{P}^T\mathbf{g})\mathbf{P}^T \cdot \mathbf{C}^\bullet + \frac{\mathbf{g}}{\rho_0\theta} \\
 & \cdot \det(\mathbf{P}^{-1})\mathbf{P}q_0(\mathbf{P}^T\mathbf{C}\mathbf{P}, \theta, \mathbf{P}^T\mathbf{g}) + \mathbf{P} \frac{\partial\psi_0}{\partial\mathbf{C}} \mathbf{P}^T \cdot \mathbf{C}^\bullet + \frac{\partial\psi_0}{\partial\theta} \cdot \theta^\bullet + \mathbf{P} \frac{\partial\psi_0}{\partial\mathbf{g}} \\
 & \cdot \mathbf{g}^\bullet + \eta_0(\mathbf{P}^T\mathbf{C}\mathbf{P}, \theta, \mathbf{P}^T\mathbf{g})\theta^\bullet \\
 & + \left( 2\mathbf{C}\mathbf{P} \frac{\partial\psi_0}{\partial\mathbf{C}} + \mathbf{g} \otimes \frac{\partial\psi_0}{\partial\mathbf{g}} + \frac{\partial\psi_c}{\partial\mathbf{g}} - \theta \frac{\partial\eta_c}{\partial\mathbf{P}} \right) \cdot (\lambda\mathbf{P}^\circ + \mathbf{P}_r^*) + \left( \frac{\partial\psi_c}{\partial\mathbf{H}} - \theta \frac{\partial\psi_c}{\partial\mathbf{H}} \right) \\
 & \cdot (\lambda\mathbf{H}^\circ + \mathbf{H}_r^*)
 \end{aligned} \tag{37}$$

We have to distinguish three cases. Firstly, if no yielding occurs and if there is no change of the thermo-kinematic state, we obtain (20) and the inequality of the viscous parts

$$0 \geq \left( 2 \mathbf{C} \mathbf{P} \frac{\partial \psi_0}{\partial \mathbf{C}} + \mathbf{g} \otimes \frac{\partial \psi_0}{\partial \mathbf{g}} + \frac{\partial \psi_c}{\partial \mathbf{P}} - \theta \frac{\partial \eta_c}{\partial \mathbf{P}} \right) \cdot \mathbf{P}'_r + \left( \frac{\partial \psi_c}{\partial \mathbf{H}} - \theta \frac{\partial \eta_c}{\partial \mathbf{H}} \right) \cdot \mathbf{H}'_r.$$

Second, if there are changes in the thermo-kinematical state, then we obtain additionally the findings (18) and (19). Third, if yielding occurs, we obtain additionally the residual inequality (21). These are again necessary and sufficient conditions for the second law.

In this extended format, the concept of elastic ranges is still applicable in the same form as in the rate-independent format. However, its name becomes now misleading, as the thermoelastic equations (1) are only fulfilled instantaneously, but not for finite processes. It should be noted that the extended format directly includes (1) the thermoelastic case (for  $\mathbf{P}'_r \equiv \mathbf{0}$ ,  $\mathbf{H}'_r \equiv \mathbf{0}$ , and  $E_p \equiv \text{Psym} \times R^+ \times V$ ), (2) a viscoelastic model of Maxwell's type ( $E_p \equiv \text{Psym} \times R^+ \times V$ ), and (3) a rate-independent elastoplastic model (for  $\mathbf{P}'_r \equiv \mathbf{0}$  and  $\mathbf{H}'_r \equiv \mathbf{0}$ ).

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