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An extended approach to multi-mechanism models in plasticity - theory and parameter identification

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Abstract

Multi-mechanism models have become an important tool for modeling of complex material behavior. In particular, two-mechanism models have been applied for modeling of ratcheting in metal plasticity as well as of steel behavior in case of phase transformations. The characteristic trait of two-mechanism models is the additive decomposition of the inelastic (i.e., plastic or visco-plastic, e.g.) strain into two or more parts (sometimes called "mechanisms") in the case of small deformations. In comparison with rheological models, there can be an interaction between these mechanisms allowing to describe important observable effects. Up to now, each mechanism has one kinematic internal variable. As a new item, we develop a framework for multi-mechanism models (in series) with several kinematic variables for each mechanism as well as with several isotropic variables for each flow criterion. In this way, the well-known "Chaboche" model with a unique inelastic strain and several kinematic variables becomes a special case of these general multi-mechanism models. Furthermore, we present a quite general approach for simulation and parameter identification based on uniaxial experiments. Finally, we give numerical examples based on cyclic experiments with the stainless steel X2CrNiMo17-12-2 (1.4404).

Contents

1 Introduction

Multi-mechanism models (abbreviated as MM models) have become an important tool for modeling complex material behavior. In applications, one encounters mostly two-mechanism models. In case of small deformations, the characteristic trait of multi-mechanism models with m mechanisms is the additive decomposition of the inelastic (i.e., plastic or visco-plastic, e.g.) strain into m parts (sometimes called "mechanisms") (see Figure 1). We refer to Saï [2011], Wolff et al. [2011b], Taleb and Cailletaud [2011], Taleb [2013] for current overviews and further references. Some new extensions can be found in Kröger [2013]. For instance, the thermoelastic strain can be regarded as a mechanism with "full rights". Moreover, evolution functionals instead of evolution equations are considered, and more complex couplings within the flow criteria are allowed. To the authors knowledge, up to now, there are only serial MM models under consideration. Multi-mechanism models in parallel with an additive split of the stress are a topic of future work (see the outlook in Subsection 6).

In comparison with rheological models (cf. Palmov [1998], Palmov [2008], e.g.), generally there can be an interaction between the (inelastic) mechanisms (within the free energy) allowing to describe important observable effects (see below for references). As a consequence of this coupling, the thermodynamic consistency of an MM model generally does not follow from the thermodynamic consistency of all its elements. On the other hand, rheological models consisting of elements connected in series are (simple) multi-mechanism models, if one element is thermoelastic. In most cases, MM models with a thermoelastic part (see Figure 1) have been studied. However, this is not a principal limitation. In Wolff et al. [2012a], Kröger et al. [2012a] and Kröger [2013], e.g., one encounters two-mechanism models without a thermoelastic element. Connecting all inelastic elements of an MM model into one inelastic element, this MM model becomes a rheological model consisting of generally two elements.
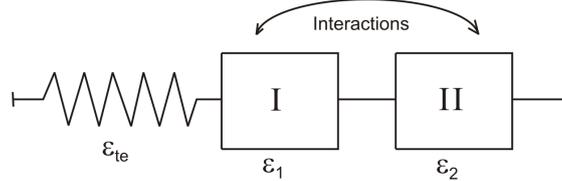
Figure 1: Scheme of a two-mechanism model. The two inelastic mechanisms I and II have their own evolution equations. Generally, they are not independent from each other. The thermoelastic strain ε_{te} is usually not regarded as a mechanism. For an alternative treatment see Kröger [2013].

If the inelastic strain is considered as one mechanism (as it was historically first), one refers to a "unified model" (or "Chaboche" model) (cf. the survey Chaboche [2008] and the references cited therein). In this case, plastic and viscous components are considered together in the same inelastic strain. In our general approach for MM models, these "Chaboche" models can be included in this framework as special MM models - as one-mechanism models. As explained in Contesti and Cailletaud [1989] and Cailletaud and Saï [1995], there are experimentally observable effects (inverse strain-rate sensibility, e.g.) which can be qualitatively correctly described by the two-mechanism approach. Moreover, this description has a plausible interpretation. To our knowledge, a first systematic formulation and investigation of two-mechanism models was given by Contesti and Cailletaud [1989].

An important application of two-mechanism models is cyclic plasticity including ratcheting. Investigations of ratcheting with the aid of two-mechanism models can be found in Saï and Cailletaud [2007], Hassan et al. [2008], Taleb and Hauet [2009], Taleb and Cailletaud [2010], Saï [2011], Taleb and Cailletaud [2011], Taleb [2013], e.g. In Hassan et al. [2008], a direct comparison between a modified Chaboche model and a 2M model has been performed (in Wolff et al. [2011b], this comparison has been

repeated in short).

Damage models combined with a multi-mechanism approach have been investigated in Besson [2009], Turki et al. [2009], Saï et al. [2011], e.g.

Another important application of two-mechanism models lies in modeling complex material behavior of steel under phase transformations. For a direct two-mechanism approach we refer to Videau et al. [1994], Aeby-Gautier and Cailletaud [2004], Wolff et al. [2008], e.g. In Wolff et al. [2011a], an algorithm for general material behavior of steel has been implemented as well as simulations have been performed, taking interaction of plasticity and transformation-induced plasticity (TRIP) into account. In Kröger [2013], a similar coupling approach has been evaluated using experimental data. There, the influence of plastic pre-deformation of austenite on the forthcoming TRIP during bainitic transformation was investigated. There are papers dealing with plasticity, visco-plasticity, transformation-induced plasticity (TRIP) and creep in steel without a coupling of these phenomena within the free energy. However, the underlying models are MM models. For instance, we refer to Mahnken et al. [2009] for plasticity and TRIP at small strains, Mahnken et al. [2012] for plasticity and TRIP at large strains, Wolff et al. [2012b] for creep and TRIP during austenitization at small strains. Contrary to the small-strain approach, in case of large deformations, there is an additive split of the velocity gradient (see Mahnken et al. [2012] and the references therein for a detailed explanation). In Mahnken et al. [2013], a multi-mechanism model for viscoplasticity at large strains has been developed, taking asymmetric effects and isotropic hardening into account. To our knowledge, up to now, there is no general theory of MM models in large strains including coupling of the kinematic variables within the free energy.

Some polymers show a material behavior similar to ratcheting in metal plasticity. This effect has been reported for an epoxy resin in Tao and Xia [2007], and in Shen et al. [2004] for epoxy polymers, e.g. In Xia et al. [2006], nonlinear viscoelastic models have been applied for the description of cyclic deformation behavior of polymers. In Wolff et al. [2012a], the two-mechanism approach has been applied to visco-elasticity with internal variables. In Kröger et al. [2012a] and Kröger et al. [2012b], a 2M model model for a rod with viscoelastic behavior has been analyzed and simulations have been performed. Mathematical results as well as simulations for an analogous $3d$ problem can be found in Kröger [2013]. Analogously as in plasticity (see Cailletaud and Saï [1995], e.g.) the two-mechanism approach can describe ratcheting effects in case of cyclic loading with non-zero mean stress.

Visco-plasticity and creep of semi-crystalline polymers in the context of multi-mechanism models have been investigated in Regrain et al. [2009] and Saï et al. [2011], e.g.

The complex material behavior of important materials (such as visco-plastic materials, shape-memory alloys, soils, granular materials, composites, biological tissues) leads to multi-mechanism models, when taking the additive decomposition of the strain tensor into account. However, in most cases, the concrete application is *not* set in the framework of multi-mechanism models. For some references see Wolff et al. [2011b].

Some current developments in MM models take considerations at the micro (meso) level into account. We refer to Saï and Cailletaud [2007], Regrain et al. [2009], Saï et al. [2011], Taleb and Hauet [2009], e.g. Here, we will not deal with this approach. However, some of the ideas pursued here can be combined with macro-micro approaches.

Multi-mechanism models are usually abbreviated by their numbers of mechanisms as well as of criteria (cf. Cailletaud and Saï [1995], e.g.). For instance, there may be $2M1C$ and $2M2C$ models. We continue this description in case of concrete given numbers. Generally, there may be n_M mechanisms and $n_C \leq n_M$ criteria. Thus, we will write "$n_M n_C$ model" or, simply as above, MM model in case no specification is needed. In the past, MM models have been applied preferably for plastic or visco-plastic behavior. However, the mechanisms may also have visco-elastic (cf. Wolff et al. [2012a], Kröger [2013], e.g.) or creep behavior (cf. Contesti and Cailletaud [1989], Wolff and Böhm [2010], e.g.). Visco-elastic and creep behavior can be regarded as phenomena with a yield stress equal to zero. Thus, there may

be common flow criteria characterized by common multipliers for the involved mechanisms. Clearly, an own criterion for each mechanism is possible, too. Plastic mechanisms are in the focus of this study. Of course, the presented general approach can be applied to other material behavior with only some specific modifications.

The main aims of this work are

- to develop a new general approach for multi-mechanism models with several mechanisms which may have several internal kinematic variables as well as with several yield criteria having several internal isotropic variables,

- to formulate general evolution laws for the internal variables which ensure thermodynamic consistency under suitable conditions,

- to develop a semi-implicit matrix-based algorithm for simulations and a parameter identification based on uniaxial experiments which is suitable for arbitrary MM models,

- to apply this algorithm to data from uniaxial experiments under cyclic loading for the stainless steel X2CrNiMo17-12-2 (1.4404).

2 Continuum-mechanical preparations

In order to have a framework for forthcoming investigations we provide some basic facts about modeling of inelastic material behavior. For comprehensive presentations of continuum mechanics we refer to Krawietz [1986], Lemaitre and Chaboche [1990], Maugin [1992], Besson et al. [2001], Haupt [2002], Bertram and Glüge [2013], e.g. We restrict ourselves to small deformations. Thus, the equation of momentum, the energy equation and the Clausius-Duhem inequality are given by

$$(2.1) \qquad \varrho_0 \, \ddot{\boldsymbol{u}} - \operatorname{div} \boldsymbol{\sigma} = \varrho_0 \boldsymbol{f},$$

$$(2.2) \qquad \varrho_0 \, \dot{e} + \operatorname{div} \boldsymbol{q} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + \varrho_0 r,$$

$$(2.3) \qquad -\varrho_0 \, \dot{\psi} - \varrho_0 \, \eta \, \dot{\theta} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\theta} \, \boldsymbol{q} \cdot \boldsymbol{\nabla}\theta \geq 0.$$

The relations (2.1) - (2.3) have to be fulfilled in the space-time domain $\Omega \times]0, T[$ ($\Omega \subset \mathbb{R}^3$ - 3d domain occupied by the body, $T > 0$ - process time). The notation is standard: ϱ_0 - density in the reference configuration, that means for $t = 0$, $\boldsymbol{u}$ - displacement vector, $\boldsymbol{\varepsilon}$ - linearized Green strain tensor, θ - absolute temperature, $\boldsymbol{\sigma}$ - Cauchy stress tensor, $\boldsymbol{f}$ - mass density of external forces, e - mass density of the internal energy, $\boldsymbol{q}$ - heat-flux density vector, r - mass density of heat supply, ψ - mass density of free (or Helmholtz) energy, η - mass density of entropy. The time derivative is denoted by a dot. $\boldsymbol{\alpha} : \boldsymbol{\beta}$ is the scalar product of the tensors, $\boldsymbol{q} \cdot \boldsymbol{p}$ is the scalar product of the vectors. We note the well-known relations

$$(2.4) \qquad \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\boldsymbol{u}) := \frac{1}{2}(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T), \qquad \psi = e - \theta \, \eta.$$

Moreover, to complete the problem, boundary and initial values must be added. For simplicity we chose the following initial values.

$$(2.5) \qquad \boldsymbol{u}(x,0) = 0, \qquad \dot{\boldsymbol{u}}(x,0) = 0, \qquad \theta(x,0) = \theta_0 \qquad \text{in } \Omega.$$

We assume mixed mechanical boundary conditions. The boundary $\partial\Omega$ is assumed to be the disjoint connection of their parts Γ_0 and Γ_1. On $\Gamma_0 \times [0, T]$ the displacement is given, here, for simplicity it is zero. On $\Gamma_1 \times [0, T]$ the traction $\boldsymbol{\tau}$ is prescribed.

$$(2.6) \qquad \boldsymbol{u} = 0 \quad \text{on } \Gamma_0 \times [0, T], \qquad \boldsymbol{\sigma}\boldsymbol{\nu} = \boldsymbol{\tau} \quad \text{on } \Gamma_0 \times [0, T].$$

(ν - outward normal on Γ_1.) The thermal boundary condition usually is given as

$$(2.7) \qquad\qquad -\boldsymbol{q}\boldsymbol{\nu} = \delta_\theta(\theta - \theta_\Gamma) \qquad\qquad\qquad \text{on } \partial\Omega \times [0, T],$$

with $\delta_\theta \geq 0$ - heat-exchange coefficient, θ_Γ - temperature of the surrounding medium.

In many cases of inelastic material behavior (in small-deformation setting), the full strain $\boldsymbol{\varepsilon}$ is split up via

$$(2.8) \qquad\qquad\qquad\qquad \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{te} + \boldsymbol{\varepsilon}_{in}$$

The thermoelastic strain $\boldsymbol{\varepsilon}_{te}$ is in functional relation with the stress $\boldsymbol{\sigma}$ (see (2.17)), $\boldsymbol{\varepsilon}_{in}$ is the inelastic strain whose evolution characterizes the behavior (plastic or creep, e.g.). Usually, in case of plastic behavior, the inelastic strain is assumed to be traceless, i.e.

$$(2.9) \qquad\qquad\qquad\qquad \text{tr}(\boldsymbol{\varepsilon}_{in}) = 0.$$

This is not a large restriction. The accumulated inelastic strain is defined by

$$(2.10) \qquad\qquad\qquad s_{in}(t) := \int_0^t (\tfrac{2}{3}\dot{\boldsymbol{\varepsilon}}_{in}(\tau) : \dot{\boldsymbol{\varepsilon}}_{in}(\tau))^{\frac{1}{2}} \, d\tau.$$

We drop the dependence on the space variable x. We propose for the free energy ψ the split

$$(2.11) \qquad\qquad\qquad\qquad \psi = \psi_{te} + \psi_{in}.$$

In case of isotropic behavior, the thermoelastic part ψ_{te} is given by (see Remark 2.1 (i) for explanations)

$$(2.12) \quad \psi_{te} := \frac{1}{2\varrho_0}\left\{2\mu\,\boldsymbol{\varepsilon}_{te} : \boldsymbol{\varepsilon}_{te} + \lambda_L(\text{tr}(\boldsymbol{\varepsilon}_{te}))^2 - 6\,K\,\alpha_\theta(\theta - \theta_0)\,\text{tr}(\boldsymbol{\varepsilon}_{te}) + 9\,K\,\alpha^2(\theta - \theta_0)^2\right\} + C(\theta).$$

Here are: $\mu > 0$ - shear modulus, $\lambda_L > 0$ - second Lamé coefficient, $K = \lambda_L + \frac{2}{3}\mu$ - compression modulus, α_θ - linear heat-dilatation coefficient, C - calorimetric function (see Helm and Haupt [2003] for explanation, e.g.). We assume that the inelastic part ψ_{in} of ψ has the general form

$$(2.13) \qquad\qquad\qquad\qquad \psi_{in} = \psi_{in}(\xi,\,\theta).$$

The quantity $\xi = (\xi_1, \ldots, \xi_{N_\xi})$ (ξ_j - scalars or tensors) represents the internal variables. Further on, these variables will be chosen in accordance with concrete models under consideration. Moreover, they have to fulfil evolution equations which are usually ordinary differential equations (ODE) with respect to the time t. We write them in the following way (see Remark 2.1 (ii) for further comments).

$$(2.14) \qquad\qquad\qquad \dot{\xi}_j = f_j^\xi(\xi, \varepsilon_{te}, \theta) \qquad\qquad\qquad \text{for } j = 1, \ldots, N_\xi.$$

As a rule, one poses zero initial conditions, i.e.

$$(2.15) \qquad\qquad\qquad \xi_j(0) = 0 \qquad\qquad\qquad\qquad \text{for } j = 1, \ldots, N_\xi.$$

Using standard arguments of thermodynamics (cf. Coleman and Gurtin [1967], Lemaitre and Chaboche [1990], Maugin [1992], Besson et al. [2001], Haupt [2002], e.g.), one obtains the *remaining inequality*

$$(2.16) \qquad\qquad\qquad \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_{in} - \varrho_0 \sum_{j=1}^{N_\xi} \frac{\partial \psi_{in}}{\partial \xi_j} : \dot{\xi}_j - \frac{1}{\theta}\,\boldsymbol{q} \cdot \boldsymbol{\nabla}\theta \geq 0.$$

as well as the potential relations

$$(2.17) \qquad \boldsymbol{\sigma} = \varrho_0 \frac{\partial \psi_{te}}{\partial \boldsymbol{\varepsilon}_{te}}, \qquad\qquad \eta = -\frac{\partial \psi}{\partial \theta}.$$

Clearly, the (isotropic) Duhamel-Neumann (i.e. generalized Hooke) relation of linear thermoelasticity results from (2.12) and (2.17).

$$(2.18) \qquad \boldsymbol{\sigma} = 2\mu\, \boldsymbol{\varepsilon}_{te} + \lambda_L \operatorname{tr}(\boldsymbol{\varepsilon}_{te})\boldsymbol{I} - 3K\alpha_\theta\,(\theta - \theta_0)\boldsymbol{I}.$$

Moreover, one defines the thermodynamic forces X_j (scalars or tensors) via

$$(2.19) \qquad X_j = \varrho_0 \frac{\partial \psi}{\partial \xi_j}, \qquad j = 1, \dots, N_\xi.$$

Usually, one assumes Fourier's law for the heat conduction

$$(2.20) \qquad \boldsymbol{q} = -\kappa_\theta\, \boldsymbol{\nabla}\theta$$

with a positive heat conductivity κ_θ (or, more generally with a positively definite heat-conductivity tensor). In case of (2.20), the heat-conduction inequality is fulfilled, i.e.

$$(2.21) \qquad -\frac{1}{\theta}\, \boldsymbol{q} \cdot \boldsymbol{\nabla}\theta \geq 0.$$

Hence, the model under consideration is *thermodynamically consistent* (see Remark 2.1 (i)), if the Clausius-Planck inequality is fulfilled

$$(2.22) \qquad \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_{in} - \sum_{j=1}^{N_\xi} X_j : \dot{\xi}_j \geq 0.$$

Up to this point, the explanations make no difference between one-mechanism models ("Chaboche" models) and n_M models. As we will see, in our extended approach, 1M models (even with multiple back stresses) are special cases of n_M models. In the theory of n_M models the following decomposition of the inelastic strain into n_M parts ("mechanisms") is crucial:

$$(2.23) \qquad \boldsymbol{\varepsilon}_{in} = \sum_{j=1}^{n_M} A_j\, \boldsymbol{\varepsilon}_j^{in}.$$

Here, the parameters A_j $(j = 1, \dots, n_M)$ are positive real numbers. However, extensions are possible regarding them as phase fractions, e.g. This approach may lead to the inclusion of effects at the micro (meso) scale. We refer to Saï and Cailletaud [2007], Saï et al. [2011]. Clearly, in this case an additional term arises in the Clausius-Planck inequality (2.22). Moreover, evolution equations for the phase fractions must be given. This is not the topic here. For further use we write ε_j^{in} instead of the widely-spread notation ε_j. As usual, the inelastic strains are traceless:

$$(2.24) \qquad \operatorname{tr}(\boldsymbol{\varepsilon}_{in}) = \operatorname{tr}(\boldsymbol{\varepsilon}_j^{in}) = 0, \qquad j = 1, \dots, n_M.$$

For all ε_j^{in} we introduce *separate* accumulations

$$(2.25) \qquad s_j(t) := \int_0^t \left(\frac{2}{3}\, \dot{\boldsymbol{\varepsilon}}_j^{in}(\tau) : \dot{\boldsymbol{\varepsilon}}_j^{in}(\tau)\right)^{\frac{1}{2}} d\tau \quad j = 1, \dots, n_M.$$

Note, that s_{in} (as defined in (2.10)) is not the sum of s_j. We introduce the local (or partial) stresses $\boldsymbol{\sigma}_j$ via

$$(2.26) \qquad \boldsymbol{\sigma}_j := A_j\, \boldsymbol{\sigma} \qquad\qquad j = 1, \dots, n_M.$$

Remarks 2.1. (i) In case of isotropy, the approach in (2.12) follows from the more general one

$$(2.27) \qquad \psi_{te} := \frac{1}{2\varrho_0} \mathbb{E}(\theta)\big(\boldsymbol{\varepsilon}_{te} - (\theta - \theta_0)\boldsymbol{G}\big) : \big(\boldsymbol{\varepsilon}_{te} - (\theta - \theta_0)\boldsymbol{G}\big) + C(\theta).$$

That means, we suppose that the mechanical part of the thermoelastic free energy is a quadratic form of the pure elastic strain $\boldsymbol{\varepsilon}_{te} - (\theta - \theta_0)\boldsymbol{G}$. The generally temperature-depending elasticity tensor of fourth order $\mathbb{E} = \mathbb{E}(\theta)$ has the following symmetry properties.

$$(2.28) \qquad \mathbb{E}_{ijkl} = \mathbb{E}_{jikl} = \mathbb{E}_{klij} \qquad\qquad \forall\, i,j,k,l \in \{1,2,3,4\}.$$

In case of full anisotropy, $\mathbb{E}$ has 21 independent entrees (cf. Haupt [2002], Bertram and Glüge [2013], e.g.). For all admissible temperatures θ the tensor $\mathbb{E}$ is positive-definite. In case of isotropy one has

$$(2.29) \qquad \mathbb{E}(\theta)\boldsymbol{\varepsilon} = 2\mu(\theta)\,\boldsymbol{\varepsilon} + \lambda_L(\theta)\mathrm{tr}(\boldsymbol{\varepsilon})\boldsymbol{I}.$$

($\mu > 0, \lambda_L$, - Lamé's coefficients, $\boldsymbol{I}$ - Identity tensor of 2nd order). $\boldsymbol{G}$ is the (symmetric) heat-dilation tensor. In case of isotropy it reads as

$$(2.30) \qquad \boldsymbol{G} = \alpha_\theta \boldsymbol{I}$$

with a linear heat-dilation coefficient α_θ. In most cases it my be assumed to be constant. In many cases, the last quadratic term in (2.12) is dropped. This does not influence the elasticity relation (2.16). The advantage of the "full" representations (2.12) and (2.27) will be evident for extensions of the model, taking damage effects into account (cf. Lemaitre and Chaboche [1990]).

(ii) The evolution equations (2.14) for the internal variables ξ_j ($j = 1, \ldots, N_\xi$) may be more general, sometimes they may (partially) implicit. More generally, they may be integral equations or general functionals (see Kröger [2013] for details). This aspect is not in the focus here. Due to (2.18), a dependence on $\boldsymbol{\sigma}$ does not consist any problem.

(iii) For concrete material models under consideration, one has to ensure that the Clausius-Planck inequality (2.22) is fulfilled for given evolution equations for $\boldsymbol{\varepsilon}_{in}$ and for ξ_j. We refer to Besson et al. [2001], Haupt [2002], e.g. for general questions, and to Wolff and Taleb [2008], Wolff et al. [2010], Wolff et al. [2011b] with respect to two-mechanism models.

(iv) By standard arguments (cf. Lemaitre and Chaboche [1990], Besson et al. [2001], Haupt [2002], e.g.), the energy equation (2.2) implies the heat-conduction equation

$$(2.31) \quad \varrho_0\, c_d\, \dot{\theta} - \mathrm{div}\,(\kappa_\theta \boldsymbol{\nabla}\theta) = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_{in} - \sum_{j=1}^{N_\xi} X_j : \dot{\xi}_j + \theta\,\frac{\partial\boldsymbol{\sigma}}{\partial\theta} : \dot{\boldsymbol{\varepsilon}}_{te} + \theta\sum_{j=1}^{N_\xi} \frac{\partial X_j}{\partial\theta} : \dot{\xi}_j + \varrho_0 r.$$

The parameter c_d is the specific heat. Here, we do not use the heat-conduction equation in data processing. In case of necessity, this equation has to be used in a suitable discretized and possibly simplified form,

3 An extended approach to multi-mechanism models

In the sequel we present *some new items* concerning kinematic as well as isotropic hardening. We investigate multi-mechanism models with n_M mechanisms and $1 \leq n_C \leq n_M$ flow criteria. As agreed in the introduction, the general abbreviation $n_M n_C$ model is used. However, in concrete cases we additionally

use the capital letters M and C. For example, we write "2M1C model" for a two-mechanism model with a common flow criterion.

In order to get a compact explanation we split up the inelastic part of the free energy ψ_{in} into two parts corresponding to kinematic and isotropic hardening, respectively:

$$(3.1) \qquad \psi_{in} = \psi_{kin} + \psi_{iso}.$$

As a consequence, here we do *not* consider a coupling between kinematic and isotropic hardening within the free energy. Otherwise, the complexity of the model would be higher. We refer to Cailletaud and Saï [1995] as well as to Wolff et al. [2010] for an example. As stated above, we focus on plastic mechanisms. We refer to Kröger [2013] for a general setting with mechanisms of different kind.

At first, we specialize the approach for the inelastic part of the free energy in (2.11), defining its part ψ_{kin} in Subsection 3.1. The part ψ_{iso} will be defined in Subsection 3.2.

3.1 Mechanisms and associated kinematic variables

We assume that each mechanism i ($i = 1, \ldots, n_M$) has $N_\alpha^{(i)}$ associated symmetric tensorial internal variables of strain type $\boldsymbol{\alpha}_j$ ($j = 1, \ldots, N_\alpha$) called "kinematic variables", where the bulk number N_α of these internal variables is given as

$$(3.2) \qquad N_\alpha := \sum_{i=1}^{n_M} N_\alpha^{(i)}.$$

The concrete relation between mechanisms and kinematic variables can be coded in a $n_M \times N_\alpha$ matrix $\mathbb{C}^\alpha$ consisting only of zeros and ones and being defined by

$$(3.3) \qquad \mathbb{C}^\alpha \in \{0,1\}^{n_M \times N_\alpha}, \qquad (\mathbb{C}^\alpha)_{ij} := \begin{cases} 1, & \text{if } \boldsymbol{\alpha}_j \text{ belongs to the mechanism } i, \\ 0, & \text{otherwise.} \end{cases}$$

The information encoded in $\mathbb{C}^\alpha$ defines two functions.
At first, each $k \in \{1, \ldots, n_M\}$ defines a set of natural numbers $\text{set}_\alpha(k)$ by

$$(3.4) \qquad \text{set}_\alpha(k) := \{j \in \{1, \ldots, N_\alpha\} \,|\, (\mathbb{C}^\alpha)_{kj} = 1\} \qquad\qquad k \in \{1, \ldots, n_M\}.$$

Since the mechanism k has $N_\alpha^{(k)}$ kinematic variables, the cardinal number of $\text{set}_\alpha(k)$ equals to $N_\alpha^{(k)}$. Moreover, $\text{set}_\alpha : \{1, \ldots, n_M\} \to 2^{\{1, \ldots, N_\alpha\}}$ is a set-valued function mapping into the set of all subsets of $\{1, \ldots, N_\alpha\}$.
On the other hand, each $i \in \{1, \ldots, N_\alpha\}$ (each variable $\boldsymbol{\alpha}_i$) belongs exactly to one $k \in \{1, \ldots, n_M\}$ (to one mechanism k). This defines the function $k_\alpha : \{1, \ldots N_\alpha\} \to \{1, \ldots n_M\}$ by

$$(3.5) \qquad k_\alpha(i) := \{k \in \{1, \ldots, n_M\} \,|\, (\mathbb{C}^\alpha)_{ki} = 1\} \qquad\qquad i \in \{1, \ldots, N_\alpha\}.$$

Remarks 3.1. (i) In Besson [2009], in connection with modeling of damage processes, several kinematic variables may be attached to one mechanism. Besides, the backstress related to the mechanism is defined in analogous way as in (3.8). However, to the authors knowledge, there is no systematic investigation in published literature.

(ii) A more descriptive interpretation of the structural matrix $\mathbb{C}^\alpha$ can be given as follows: Each of the N_α columns has exactly one entry with "1" belonging to the row which describes the corresponding mechanism. This fact is expressed by the function k_α in (3.5). On the other hand, each of the n_M rows has exactly $N_\alpha^{(k)}$ entries with "1" belonging to the columns which describe the associated kinematic variables. This fact is expressed by the set-valued function set_α.

(iii) The mechanisms and kinematic variables may be arranged in such an order, that the first row stands for the first mechanism and its associated variables occupy the first $N_\alpha^{(1)}$ columns, etc. For more clarity, the following formula shows the arrangement of tensorial internal variables $\boldsymbol{\alpha}_j$ in this special case.

$$(3.6) \qquad \underbrace{\alpha_1, \alpha_2, \ldots, \alpha_{N_\alpha^{(1)}}}_{1^{st} \text{ mechanism}}, \underbrace{\alpha_{N_\alpha^{(1)}+1}, \ldots, \alpha_{N_\alpha^{(1)}+N_\alpha^{(2)}}}_{2^{nd} \text{ mechanism}}, \cdots$$

$$\cdots, \underbrace{\alpha_{N_\alpha^{(1)}+N_\alpha^{(2)}+\cdots+N_\alpha^{(n_M-1)}+1}, \ldots, \alpha_{N_\alpha^{(1)}+N_\alpha^{(2)}+\cdots+N_\alpha^{(n_M)}}}_{n_M^{th} \text{ mechanism}}.$$

Note, that in this case the set $\text{set}_\alpha(k)$ is an interval consisting of $N_\alpha^{(k)}$ numbers. The forthcoming considerations do not depend on a special arrangements of the rows and columns like in (3.6). However, the presentation in this manner may be more convenient.

(iv) The matrix-based approach shows its advantage when preparing and performing numerical simulations. We will deal with this in Section 4.

We assume for the part ψ_{kin} of the free energy (cf. (3.1))

$$(3.7) \qquad \psi_{kin}(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_{N_\alpha}, \theta) := \frac{1}{3\varrho_0} \sum_{i,j=1}^{N_\alpha} c_{ij}(\theta)\, \boldsymbol{\alpha}_i : \boldsymbol{\alpha}_j.$$

Without any loss of generality we assume that the matrix $\boldsymbol{c} = (c_{ij})$ is symmetric. In a usual way we define the back stresses $\overline{\boldsymbol{X}}_i$ ($i = 1, \ldots, N_\alpha$) as thermodynamic forces related to the kinematic internal variables $\boldsymbol{\alpha}_i$ in accordance with (2.19) by

$$(3.8) \qquad \overline{\boldsymbol{X}}_i = \varrho_0 \frac{\partial \psi_{kin}}{\partial \boldsymbol{\alpha}_i} = \frac{2}{3} \sum_{j=1}^{N_\alpha} c_{ij}\, \boldsymbol{\alpha}_j, \qquad\qquad i = 1, \ldots, N_\alpha.$$

The factors $\frac{1}{3}$ in (3.7) and $\frac{2}{3}$ in (3.8) ensure a compatibility between $3d$ and $1d$ representations of the corresponding formulas. We need this in simulations and applications (cf. Subsection 4.1).

We sum up all back stresses $\overline{\boldsymbol{X}}_i$ belonging to the same mechanism, defining back stresses $\boldsymbol{X}_k$ ($k = 1, \ldots, n_M$) associated with the kth mechanism by

$$(3.9) \qquad \boldsymbol{X}_k = \sum_{i \in \text{set}_\alpha(k)} \overline{\boldsymbol{X}}_i \qquad\qquad k = 1, \ldots, n_M,$$

or, equivalently in short

$$(3.10) \qquad\qquad\qquad \boldsymbol{X} = \mathbb{C}^\alpha\, \overline{\boldsymbol{X}}$$

with the obvious definitions $\boldsymbol{X} := \{\boldsymbol{X}_1, \ldots, \boldsymbol{X}_{n_M}\}$ and $\overline{\boldsymbol{X}} := \{\overline{\boldsymbol{X}}_1, \ldots, \overline{\boldsymbol{X}}_{N_\alpha}\}$. The back stresses $\boldsymbol{X}_k$ ($k = 1, \ldots, n_M$) are related to the mechanism in a one-to-one manner. Moreover, they are involved in the evolution equations of the mechanisms (see formulas (3.49), (3.53), e.g.).

We assume that for each fixed temperature θ (at least of the admissible domain) the (symmetric) matrix $\boldsymbol{c} = (c_{ij})$ is positive semi-definite, i.e. there holds

$$(3.11) \qquad \forall\, \xi \in \mathbb{R}^{N_\alpha} \qquad\qquad : \qquad\qquad \sum_{i,j=1}^{N_\alpha} c_{ij}(\theta)\xi_i\xi_j \geq 0.$$

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Under the condition (3.11) ψ_{kin} is a convex function with respect to $\{\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_{N_\alpha}\}$. We demand (cf. Remark 3.2 (ii) for explanations)

$$(3.12) \qquad \forall\, i \in \{1, \ldots, N_\alpha\} \qquad\qquad : \qquad\qquad c_{ii} > 0.$$

To our knowledge, the general approach of multi-mechanism models with multiple kinematic variables for one mechanism is *new*. It covers multi-mechanism models in use as well as 1M models. We give three examples.

3.1.1 Current state of multi-mechanism models

Up to now, MM models with the *same* number of mechanisms and tensorial internal variables of strain type have been investigated and applied (see Cailletaud and Saï [1995], Taleb and Cailletaud [2010], Saï [2011], Wolff et al. [2011b], e.g.). In this case, all numbers $N_\alpha^{(i)}$ are equal to one, and $n_M = N_\alpha$, and the structural matrix $\mathbb{C}^\alpha$ is the $n_M \times n_M$ identity matrix, and it does not contain any additional information. It suffices to determine the number of mechanisms n_M. Clearly, in this case there holds

$$(3.13) \qquad \boldsymbol{X}_k = \overline{\boldsymbol{X}}_k \qquad\qquad k = 1, \ldots, n_M.$$

3.1.2 One-mechanism models ("Chaboche" models)

The approach in (3.3) and (3.7) generalizes 1M models with *several* back stresses with their own evolutions. These models are called "Chaboche" models, and they are used for modeling plastic and visco-plastic behavior. We refer to Chaboche [2008], Abdel-Karim [2010], Desmorat [2010], e.g. Indeed, for a 1M model with N_α^1 tensorial internal variables of strain type, one has $n_M = 1$, and the bulk back stress $\boldsymbol{X}_1 = \boldsymbol{X}$ is given by

$$(3.14) \qquad \boldsymbol{X} = \sum_{i=1}^{N_\alpha^1} \overline{\boldsymbol{X}}_i.$$

Moreover, the structural matrix $\mathbb{C}^\alpha$ consists of one row with N_α^1 entries being equal to one. In this case, the matrix $\mathbb{C}^\alpha$ also does not contain any additional information. It suffices to determine the number of partial back stresses N_α^1. In applications to ratcheting, the number N_α^1 frequently is 4, sometimes 8 (cf. Taleb and Cailletaud [2010], Abdel-Karim [2010], e.g.).

3.1.3 A prototypical example of the extended approach

Clearly, the number of parameters c_{ij} in (3.7) can quickly growth in the general case. Hence, to keep track of this general case, we consider a simple version: A 2M model where the first mechanism has *two* variables $\boldsymbol{\alpha}$, while the second mechanism has only one kinematic variable. Thus, the structural matrix $\mathbb{C}^\alpha$ reads as

$$(3.15) \qquad \mathbb{C}^\alpha = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Moreover, the symmetric 3×3 matrix $\boldsymbol{c}$ defining the part of the free energy ψ_{kin} is described by six coefficients which are arranged as follows.

$$(3.16) \qquad \boldsymbol{c} = \left(\begin{array}{cc|c} c_{11} & c_{12} & c_{13} \\ c_{12} & c_{22} & c_{23} \\ \hline c_{13} & c_{23} & c_{33} \end{array} \right), \qquad \boldsymbol{c}_I = \begin{pmatrix} c_{11} & c_{12} \\ c_{12} & c_{22} \end{pmatrix}, \qquad \boldsymbol{c}_{II} = \begin{pmatrix} c_{33} \end{pmatrix}$$

The first mechanism has the two internal variables, $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$. The variable $\boldsymbol{\alpha}_3$ belongs to the second mechanism. The sub-matrix $\boldsymbol{c}_I$ corresponds to the first mechanism, and the interaction inside of this mechanism is described by c_{12}. The sub-matrix $\boldsymbol{c}_{II}$ is assigned to the second mechanism. The coefficients c_{13} and c_{23} describe interactions between the two mechanisms. Specializing the formulas (3.8) and (3.9), we get

$$(3.17) \qquad \overline{\boldsymbol{X}}_i = \frac{2}{3} \sum_{j=1}^{3} c_{ij}\, \boldsymbol{\alpha}_j, \qquad\qquad i = 1, 2, 3,$$

$$(3.18) \qquad \boldsymbol{X}_1 = \overline{\boldsymbol{X}}_1 + \overline{\boldsymbol{X}}_2, \qquad\qquad \boldsymbol{X}_2 = \overline{\boldsymbol{X}}_3$$

In the sequel, we will use this example as a reference example in order to demonstrate the possibilities of the general approach.

Remarks 3.2. Some items concerning symmetric matrices

(i) It follows from algebraic considerations, that the sum in (3.7) is non-negative for all symmetric 3×3 matrixes $\boldsymbol{\alpha}_i$ ($i = 1, \ldots, N_\alpha$), if and only if (3.11) is fulfilled. Besides, the convexity of ψ_{kin} follows in this case.

(ii) From the positive semi-definiteness of the matrix $\boldsymbol{c}$ the inequalities

$$(3.19) \qquad \forall\, i \in \{1, \ldots, N_\alpha\} \quad : \quad c_{ii} \geq 0$$

follow. Moreover, if there is $c_{ij} = 0$ for one pair of indices (i, j), then all entries in the ith row and in the jth colon are zero. Thus, it is reasonable to assume the condition (3.12).

(iii) The matrix $\boldsymbol{c}$ is called "positive definite", if the sum in (3.11) is positive for all non-vanishing $\xi \in \mathbb{R}^{N_\alpha}$. In this case, the determinant $\det(\boldsymbol{c})$ is not zero, and the matrix $\boldsymbol{c}$ is invertible.

(iv) For a symmetric 2×2 matrix $\boldsymbol{c}$ positive semi-definiteness is equivalent to the condition

$$(3.20) \qquad c_{12}^2 \leq c_{11}c_{22}.$$

Moreover, positive definiteness is equivalent to the strong inequality in (3.20) (see Wolff and Taleb [2008], e.g.).

3.2 Flow criteria and associated isotropic variables

As already stated above, an n_M model may have $1 \leq n_C \leq n_M$ flow criteria. We assume that the ith ($i \in \{1, \ldots, n_C\}$) criterion is related to $N_f^{(i)}$ ($i = 1, \ldots, n_C$) mechanisms. In other words, the $N_f^{(i)}$ ($i = 1, \ldots, n_C$) mechanisms have the ith criterion as their common one. Of course, the special cases of one-criterion models (1C models) as well as of $n_M n_M$ models are covered, too. In the first case, one has $N_f^{(1)} = n_M$. In the second case, all numbers $N_f^{(i)}$ are equal to one. Clearly, there must be

$$(3.21) \qquad \sum_{j=1}^{n_C} N_f^{(j)} = n_M.$$

In an analogous way as for mechanisms and kinematic variables in the previous Subsection, the concrete relations between mechanisms and flow criteria can be coded by a structural $n_C \times n_M$ matrix $\mathbb{C}^f$:

$$(3.22) \qquad \mathbb{C}^f \in \{0, 1\}^{n_C \times n_M}, \qquad (\mathbb{C}^f)_{ij} := \begin{cases} 1, & \text{if mechanism } j \text{ belongs to the criterion } i, \\ 0, & \text{otherwise.} \end{cases}$$

Again (cf. (3.4)), the information encoded in the matrix $\mathbb{C}^f$ defines two functions: At first, a set-valued function $\text{set}_f : \{1, \ldots, n_C\} \to 2^{\{1, \ldots, n_M\}}$ is given by

$$(3.23) \qquad \text{set}_f(k) := \{j \in \{1, \ldots, n_M\} \,|\, (\mathbb{C}^f)_{kj} = 1\} \qquad\qquad k \in \{1, \ldots, n_C\}.$$

Secondly, a function $k_f : \{1, \ldots, n_M\} \to \{1, \ldots, n_C\}$ is defined by

$$(3.24) \qquad k_f(i) := \{k \in \{1, \ldots, n_C\} \,|\, (\mathbb{C}^f)_{ki} = 1\} \qquad\qquad i \in \{1, \ldots, n_M\}.$$

We assume that $N_q^{(i)}$ isotropic internal variables q_j are associated to the ith criterion ($i \in \{1, \ldots, n_C\}$). Hence, the number of all isotropic internal variable is given by

$$(3.25) \qquad\qquad\qquad N_q := \sum_{i=1}^{nuc} N_q^{(i)}.$$

Again, the concrete relation between flow criteria and isotropic variables can be coded via a structural $n_C \times N_q$ matrix $\mathbb{C}^q$:

$$(3.26) \qquad \mathbb{C}^q \in \{0,1\}^{n_C \times N_q}, \qquad (\mathbb{C}^q)_{ij} := \begin{cases} 1, & \text{if } q_j \text{ belongs to the flow criterion } i, \\ 0, & \text{otherwise.} \end{cases}$$

Again (cf. (3.4) and vv), the information encoded in the matrix $\mathbb{C}^q$ defines two functions: At first, a set-valued function $\text{set}_q : \{1, \ldots, n_C\} \to 2^{\{1, \ldots, N_q\}}$ is given by

$$(3.27) \qquad \text{set}_q(k) := \{j \in \{1, \ldots, N_q\} \,|\, (\mathbb{C}^q)_{kj} = 1\} \qquad\qquad k \in \{1, \ldots, n_C\}.$$

Secondly, a function $k_q : \{1, \ldots, N_q\} \to \{1, \ldots, n_C\}$ is defined by

$$(3.28) \qquad k_q(i) := \{k \in \{1, \ldots, n_C\} \,|\, (\mathbb{C}^q)_{ki} = 1\} \qquad\qquad i \in \{1, \ldots, N_q\}.$$

Remark 3.3. Obviously, there hold analogous remarks concerning the matrices $\mathbb{C}^f$ and $\mathbb{C}^q$ like for the matrix $\mathbb{C}^\alpha$ in the Remarks 3.1.

Now we assume for the part ψ_{iso} (see (3.1))

$$(3.29) \qquad\qquad \psi_{iso}(q_1, \ldots, q_{N_q}, \theta) := \frac{1}{2\varrho_0} \sum_{i,j=1}^{N_q} Q_{ij} \, q_i q_j.$$

The part ψ_{kin} remains the same as in (3.7). In analogy to the matrix $\boldsymbol{c}$ we assume that for each fixed temperature θ (at least of the admissible domain) the following condition holds.

$$(3.30) \qquad \forall \xi \in \mathbb{R}^{N_q} \qquad\qquad : \qquad\qquad \sum_{i,j=1}^{N_q} Q_{ij}(\theta) \xi_i \xi_j \geq 0.$$

Without any loss of generality the matrix $\boldsymbol{Q}$ can be assumed to be symmetric. As above for the matrix $\boldsymbol{c}$ (cf. Remark 3.2 (i)) it is reasonable to assume

$$(3.31) \qquad \forall\, i \in \{1, \ldots, N_q\} \qquad\qquad : \qquad\qquad Q_{ii}(\theta) > 0.$$

The isotropic hardening stresses $\overline{R}_i$ are defined in accordance with the general approach in (2.19). Hence, one has

$$(3.32) \qquad \overline{R}_i = \varrho_0 \frac{\partial \psi_{iso}}{\partial q_i} = \sum_{j=1}^{N_q} Q_{ij} \, q_j \qquad\qquad i \in \{1, \ldots, N_q\},$$

Sometimes, in the case of 1C models with only one isotropic variable, instead of q_1, Q_{11} and $\overline{R}_1$ one simply writes q, Q and R, respectively. Analogously as in the case of kinematic hardening, we sum up all isotropic hardening stresses belonging to the same criterion, defining

$$(3.33) \qquad R_k = \sum_{i \in \mathrm{set}_q(k)} \overline{R}_i \qquad\qquad k = 1, \ldots, n_C.$$

The last relation can be expressed in an equivalent way:

$$(3.34) \qquad\qquad \boldsymbol{R} = \mathbb{C}^q\, \overline{\boldsymbol{R}}$$

with $\boldsymbol{R} := (\boldsymbol{R}_1, \ldots, \boldsymbol{R}_{n_C})$ and $\overline{\boldsymbol{R}} := (\overline{\boldsymbol{R}}_1, \ldots, \overline{\boldsymbol{R}}_{N_q})$. The quantities R_k are related to the flow criteria in a one-to-one manner.

Based on the von Mises stress, we define the quantities

$$(3.35) \qquad \overline{J}_i := \left(\frac{3}{2} (\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*) : (\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*) \right)^{\frac{1}{2}} \qquad i = 1, \ldots, n_M,$$

$$(3.36) \qquad J_k := \left(\sum_{i \in \mathrm{set}_f(k)} \overline{J}_i^{\beta} \right)^{\frac{1}{\beta}} \qquad k = 1, \ldots, n_C.$$

The quantity $\boldsymbol{\sigma}^*$ stands for the deviator of $\boldsymbol{\sigma}$, and $\overline{J}_i$ can be regarded as the von Mises stress of the "effective stress" of the ith mechanism. The quantity J_k is some kind of "effective stress" associated with the kth criterion. The material parameter β has to fulfil

$$(3.37) \qquad\qquad \beta > 1.$$

Frequently, the parameter β is labelled by N, see Wolff and Taleb [2008], Taleb and Cailletaud [2010]. More comments can be found in Remarks 3.4 (ii), (iii).

The definition (3.36) of the von Mises stresses $\boldsymbol{J} := (J_1, \ldots, J_{n_C})$ related to the flow criteria can be expressed in a compact way.

$$(3.38) \qquad\qquad \boldsymbol{J} = \left(\mathbb{C}^f\, \overline{\boldsymbol{J}}^{\beta} \right)^{\frac{1}{\beta}}$$

with $\overline{\boldsymbol{J}} := (\overline{J}_1, \ldots, \overline{J}_{n_M})$. The power operations in (3.38) are understood in a *component-wise* way.

Generally, there are more mechanisms than flow criteria, i.e. $n_C \leq n_M$. Thus, for technical reason in the sequel, we define an auxiliary vector $\boldsymbol{J}^{(m)}$ of von Mises stresses related to the mechanisms by:

$$(3.39) \qquad\qquad \boldsymbol{J}^{(m)} := \left(\mathbb{C}^f \right)^T \boldsymbol{J}.$$

$\left(\mathbb{C}^f \right)^T$ is the transposed matrix to $\mathbb{C}^f$. Clearly, in general case, some components of $\boldsymbol{J}^{(m)}$ are equal, however, the number of components is equal to the number of mechanisms n_M.

The yield functions are given by

$$(3.40) \qquad f_k(\boldsymbol{\sigma}_i, \boldsymbol{X}_i, R_k, R_{0k}) := J_k - (R_k + R_{0k}) \qquad k = 1, \ldots, n_C, \quad i \in \mathrm{set}_f(k),$$

$$(3.41) \qquad R_{0k} := \sqrt[\beta]{N_f^{(k)}}\, \sigma_{0k}, \qquad k = 1, \ldots, n_C.$$

The quantities $\sigma_{0k} = \sigma_{0k}(\theta) > 0$ ($i = 1, \ldots, n_C$) are the initial yield stresses associated with the corresponding flow criteria. It is assumed that

$$(3.42) \qquad\qquad \sigma_{0k}(\theta) > 0 \qquad \text{for } k = 1, \ldots, n_C.$$

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The notation in (3.40) means that the kth flow function f_k depends on all $\boldsymbol{\sigma}_i$ and $\boldsymbol{X}_i$ which mechanisms i are united by the kth flow criterion.

In order to have formally the same number of flow criteria and mechanisms, we define a new vector of flow functions $\boldsymbol{f}^{(m)}$ by

$$(3.43) \qquad \boldsymbol{f}^{(m)} := \left(\mathbb{C}^f\right)^T \boldsymbol{f},$$

whereby $\boldsymbol{f} := (f_1, \ldots, f_{n_C})$ and the f_k are defined in (3.40), (3.41).

Since we are dealing only with plastic behavior, we suppose for all $n_M n_C$ models the subsequent n_C constraints

$$(3.44) \qquad f_k(\boldsymbol{\sigma}_i, \boldsymbol{X}_i, R_k, R_{0k}) \leq 0 \qquad\qquad k = 1, \ldots, n_C, \qquad\qquad i \in \mathrm{set}_f(k),$$

or, in short, using (3.43)

$$(3.45) \qquad \boldsymbol{f}^{(m)}(\boldsymbol{\sigma}_{(A)}, \boldsymbol{X}, \boldsymbol{R}, \boldsymbol{R}_0) \leq 0$$

with the vector $\boldsymbol{\sigma}_{(A)}$ of partial stresses defined by

$$(3.46) \qquad \sigma_{(A)} := (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_{n_M}).$$

Remarks 3.4. (i) In Taleb and Cailletaud [2010], the isotropic hardening R is represented as a sum of two parts having their own evolutions and involving additional variables. The aim is to obtain a better description of ratcheting. This approach is analogous to the representation of one back stress as a sum of partial back stresses as in (3.9).

(ii) In the case $n_M = n_C$ each mechanism has its own flow criterion, and, from (3.35), (3.36) follows

$$(3.47) \qquad \overline{J}_i = J_i = \left(\frac{3}{2}(\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*) : (\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*)\right)^{\frac{1}{2}} \qquad \text{for } i = 1, \ldots, n_M.$$

Therefore, there is no parameter β in this case. Similarly, for 1M models ("Chaboche" models) one has $J_1 = \overline{J}_1$, and the parameter β does not play any role, too.

(iii) In case of $n_C = 1$, all mechanisms have a common flow criterion, and (3.35), (3.36) yield

$$(3.48) \qquad J = \left(\sum_{i=1}^{n_M} \overline{J}_i^\beta\right)^{\frac{1}{\beta}}.$$

(iv) A current proposal for a more complex coupling between the mechanisms via the flow criteria can be found in Kröger [2013].

3.3 Evolution equations for inelastic strains

Based on (3.35) and (3.36), we define

$$(3.49) \qquad \boldsymbol{n}_i := -\frac{\partial f_k}{\partial \boldsymbol{X}_i} = \frac{3}{2}\frac{\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*}{\overline{J}_i}\left(\frac{\overline{J}_i}{J_k}\right)^{\beta-1} \qquad k = 1, \ldots, n_C, \qquad i \in \mathrm{set}_f(k).$$

Using the definitions in (3.38) and (3.39), the definition (3.49) reads as

$$(3.50) \qquad \boldsymbol{n}_i = \frac{3}{2}\frac{\boldsymbol{\sigma}_i^* - \boldsymbol{X}_i^*}{\overline{J}_i}\left(\frac{\overline{J}_i}{J_i^{(m)}}\right)^{\beta-1} \qquad\qquad i = 1, \ldots, n_M.$$

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Moreover, using the vector $\boldsymbol{n} := (\boldsymbol{n}_1, \ldots, \boldsymbol{n}_{n_M})$ the last relation can be re-written in a compact way (see (3.46) for the definition of $\boldsymbol{\sigma}_{(A)}$).

$$(3.51) \qquad \boldsymbol{n} = \frac{3}{2} \frac{\boldsymbol{\sigma}^*_{(A)} - \boldsymbol{X}^*}{\overline{\boldsymbol{J}}} \left(\frac{\overline{\boldsymbol{J}}}{\boldsymbol{J}^{(m)}} \right)^{\beta - 1}.$$

Again, the algebraic operations are understood in a component-wise manner.

For further use, we introduce unit tensors $\boldsymbol{m}_i$ being collinear to $\boldsymbol{n}_i$ as well as to to the effective stresses of the ith mechanisms.

$$(3.52) \qquad \boldsymbol{m}_i := \boldsymbol{n}_i \, \|\boldsymbol{n}_i\|^{-1} = \frac{\boldsymbol{\sigma}^*_i - \boldsymbol{X}^*_i}{\|\boldsymbol{\sigma}^*_i - \boldsymbol{X}^*_i\|} \qquad\qquad i = 1, \ldots, n_M.$$

Now we assume evolution laws for ε_i. All mechanisms belonging to the same flow criterion have a common plastic multiplier. Thus, we assume

$$(3.53) \qquad \dot{\boldsymbol{\varepsilon}}_i^{in} = \lambda_k \, \boldsymbol{n}_i, \qquad\qquad k = 1, \ldots, n_C, \qquad\qquad i \in \mathrm{set}_f(k).$$

As usual, the plastic multipliers λ_k have to fulfil

$$(3.54) \qquad \lambda_k \begin{cases} = 0, & \text{if} \quad f_k(\boldsymbol{\sigma}_i, \boldsymbol{X}_i, R_k, R_{0k}) < 0, \\ \geq 0, & \text{if} \quad f_k(\boldsymbol{\sigma}_i, \boldsymbol{X}_i, R_k, R_{0k}) = 0. \end{cases} \qquad k = 1, \ldots, n_C \quad i \in \mathrm{set}_f(k).$$

In applications, it may be useful to re-write the relations (3.53) and (3.54) in a compact matrix-based way. For this reason, we define suitable vectors stemming from the vector $\boldsymbol{\lambda} := (\lambda_1, \ldots, \lambda_{nuc})$ of plastic multipliers.

$$(3.55) \qquad \boldsymbol{\lambda}^{(q)} := \left(\mathbb{C}^q \right)^T \boldsymbol{\lambda}, \qquad\quad \boldsymbol{\lambda}^{(m)} := \left(\mathbb{C}^f \right)^T \boldsymbol{\lambda}, \qquad\quad \boldsymbol{\lambda}^{(\alpha)} := \left(\mathbb{C}^\alpha \right)^T \left(\mathbb{C}^f \right)^T \boldsymbol{\lambda}.$$

Therefore, the evolution equations for the vector $\boldsymbol{\varepsilon}_{(m)}^{in} := (\varepsilon_1^{in}, \ldots, \varepsilon_{num}^{in})$ of partial plastic strain reads as (cf. (3.53))

$$(3.56) \qquad \dot{\boldsymbol{\varepsilon}}_{(m)}^{in} = \boldsymbol{\lambda}^{(m)} \, \boldsymbol{n}.$$

Again, the multiplication on the right-hand side is component-wise. The flow conditions (3.54) can be re-formulated equivalently in the following compact way using the Kuhn-Tucker conditions.

$$(3.57) \qquad \boldsymbol{\lambda}^{(m)} \geq 0, \qquad \boldsymbol{f}^{(m)}(\boldsymbol{\sigma}_{(A)}, \boldsymbol{X}, R, R_0) \leq 0, \qquad \boldsymbol{\lambda}^{(m)} \boldsymbol{f}^{(m)}(\boldsymbol{\sigma}_{(A)}, \boldsymbol{X}, R, R_0) = 0.$$

Clearly, the order relations have to be understood component-wise.

From (2.25), (3.35), (3.36), (3.49) and (3.53) one gets

$$(3.58) \qquad \dot{s}_i = \lambda_k \left(\sum_{j \in \mathrm{set}_f(k)} \overline{J}_j^\beta \right)^{\frac{1}{\beta} - 1} \overline{J}_i^{\beta - 1} \qquad\qquad k = 1, \ldots, n_C, \qquad\qquad i \in \mathrm{set}_f(k),$$

and, after this,

$$(3.59) \qquad \lambda_k = \left(\sum_{j \in \mathrm{set}_f(k)} (\dot{s}_j)^{\frac{\beta}{\beta - 1}} \right)^{\frac{\beta - 1}{\beta}}, \qquad\qquad k = 1, \ldots, n_C.$$

In case of necessity, the last two relations can be re-written in a compact way, too.

3.4 Evolution equations for isotropic variables and isotropic hardening stresses

We assume the following evolution equations for q_i.

$$(3.60) \qquad \dot{q}_i = \lambda_{k_q(i)} - \bar{b}_i(\overline{\boldsymbol{R}}, \boldsymbol{q}, \boldsymbol{\lambda}, \theta, \boldsymbol{\sigma}) \qquad\qquad i = 1, \ldots, N_q.$$

The $\bar{b}_i$ are given functions depending on the quoted quantities and possibly on further ones like accumulations. The vectorial notations $\overline{\boldsymbol{R}}$, $\boldsymbol{q}$ and $\boldsymbol{\lambda}$ stand for the sets of all R_i, q_i and λ_k, respectively. The evolution equations (3.60) cover many approaches in use. It is inspired by an analogous general approach which has been investigated in Desmorat [2010] for kinematic variables in the case of 1M models (see below). Appropriate conditions on the functions $\bar{b}_i$ ensure thermodynamic consistency. This will be considered in Subsection 3.6.

Here, in case of plastic behavior, the following restriction ensures that the evolution of q_i can only take place, if the corresponding flow criterion is fulfilled. This can be expressed by

$$(3.61) \qquad \lambda_{k_q(i)} = 0 \quad \Rightarrow \quad \bar{b}_i = 0 \qquad i = 1, \ldots, N_q.$$

Using (3.60) and the definition of the isotropic hardening stresses R_i in (3.32), general evolution equations for R_i follow.

$$(3.62) \qquad \overline{\dot{R}}_i = \sum_{j=1}^{N_q} Q_{ij} \lambda_{k_q(j)} - \sum_{j=1}^{N_q} Q_{ij} \bar{b}_j(\overline{\boldsymbol{R}}, \boldsymbol{q}, \boldsymbol{\lambda}, \theta, \boldsymbol{\sigma}) + \dot{\theta} \sum_{j=1}^{N_q} \frac{\mathrm{d}Q_{ij}}{\mathrm{d}\theta} q_j \qquad i = 1, \ldots, N_q.$$

In the *regular* case $\det(\boldsymbol{Q}) \neq 0$, $\boldsymbol{Q}$ is invertible, and the equations (3.62) can be re-formulated without q_j. For a *constant* matrix $\boldsymbol{Q}$, the equations (3.62) do not contain the last sum with q_j. Finally, from (3.33) the equations for the isotropic hardening stresses R_i associated with the criteria follow.

$$(3.63) \qquad \dot{R}_k = \sum_{i \in \mathrm{set}_q(k)} \overline{\dot{R}}_i \qquad\qquad k = 1, \ldots, n_C,$$

or, in short (cf. (3.34))

$$(3.64) \qquad \dot{\boldsymbol{R}} = \mathbb{C}^q \, \overline{\dot{\boldsymbol{R}}}.$$

An important special case of the general approach in (3.60) is given by

$$(3.65) \qquad \dot{q}_i = \lambda_{k_q(i)} - \sum_{j=1}^{N_q} b_{ij} \overline{R}_j \sqrt{\lambda_{k_q(j)}} \sqrt{\lambda_{k_q(i)}} \qquad\qquad i = 1, \ldots, N_q,$$

where $\boldsymbol{b}$ is a not necessarily symmetric matrix of material parameters generally depending on temperature and further quantities. Now the evolution equations for $\overline{R}_i$ become

$$(3.66) \qquad \overline{\dot{R}}_i = \sum_{j=1}^{N_q} Q_{ij} \lambda_{k_q(j)} - \sum_{j,s=1}^{N_q} Q_{ij} b_{js} \overline{R}_s \sqrt{\lambda_{k_q(s)}} \sqrt{\lambda_{k_q(j)}} + \dot{\theta} \sum_{j=1}^{N_q} \frac{\mathrm{d}Q_{ij}}{\mathrm{d}\theta} q_j \qquad i = 1, \ldots, N_q.$$

In order to re-formulate the evolution equations (3.65) for $\boldsymbol{q} = (q_1, \ldots, q_{N_q})$ and (3.66) for $\overline{\boldsymbol{R}} = (\overline{R}_1, \ldots, \overline{R}_{N_q})$, we define special diagonal matrices.

$$(3.67) \qquad \Lambda^{(q)} \in \mathbb{R}^{N_q \times N_q}, \qquad\qquad \Lambda^{(q)} := diag\{(\mathbb{C}^q)^T \sqrt{\boldsymbol{\lambda}}\}.$$

The operation $diag\{\boldsymbol{v}\}$ generates a quadratic diagonal matrix from a given vector $\boldsymbol{v}$. The square root in the middle of (3.67) is understood as a component-wise operation. Thus, an *equivalent* definition for $\Lambda^{(q)}$ is given by

$$(3.68) \qquad \Lambda^{(q)} \in \mathbb{R}^{N_q \times N_q}, \qquad\qquad (\Lambda^{(q)})_{ij} := \left\{ \begin{array}{ll} \sqrt{\lambda_i^{(q)}}, & \text{if } i = j, \\ 0, & \text{otherwise.} \end{array} \right. .$$

As a result, the evolutions equation (3.65) and (3.66) can be re-written as follows.

$$(3.69) \qquad \dot{\boldsymbol{q}} = \boldsymbol{\lambda}^{(q)} - \Lambda^{(q)} \boldsymbol{b} \Lambda^{(q)} \overline{R},$$

$$(3.70) \qquad \dot{\overline{R}} = \boldsymbol{Q}\Big(\boldsymbol{\lambda}^{(q)} - \Lambda^{(q)} \boldsymbol{b} \Lambda^{(q)} \overline{R}\Big) + \dot{\theta}\big(\frac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}\theta}\big)\boldsymbol{q},$$

Remarks 3.5. (i) (**One-criterion models with one isotropic variable**) The general approach in (3.60) as well in (3.65) covers well-known cases. For instance, in case of 1C models with one isotropic variable, the equations (3.65) turn to one equation sometimes written in the following form

$$(3.71) \qquad \dot{q} = \lambda - \frac{b}{Q} R\lambda.$$

with $b \geq 0$. Due to (3.32) and $Q > 0$, now q can always be eliminated. Hence, the pendant to (3.62) reads as

$$(3.72) \qquad \dot{R} = Q\lambda - bR\lambda + \frac{\dot{\theta}}{Q}\frac{\mathrm{d}Q}{\mathrm{d}\theta}R.$$

For *constant* Q and $b > 0$ and the for the usual initial condition $R(0) = 0$ the solution of (3.72) is given by

$$(3.73) \qquad R(\Lambda) = \frac{Q}{b}\big(1 - \exp(-b\Lambda)\big)$$

with (cf. (2.10) and (3.58))

$$(3.74) \qquad \Lambda(t) := \int_0^t \lambda(\tau)\,\mathrm{d}\tau = s(t)$$

The curve given by (3.73) describes clearly the isotropic hardening with saturation. The initial sloop of this curve is Q, while its asymptotic value is Q/b.

In the special case of 1C models with one isotropic variable and with (3.71), in accordance to (3.73), the isotropic hardening stress R is a non-negative function of the plastic accumulation Λ.

In the general situation (3.60) or (3.65), it is a mathematical task to investigate under which conditions on $\bar{b}_i$ (or on b_{ij}) the quantities R_k are non-negative.

(ii) In non-isothermal situation, rate-independence of isotropic hardening is ensured under condition (3.61) *and* if the matrix $\boldsymbol{Q}$ is constant.

3.5 Evolution equations for kinematic variables and back stresses

Analogously as for isotropic hardening, we present a general variant of evolution equations for the kinematic variables which generalizes many approaches in use. In particular, this approach contains the case

of 1M models which has been investigated in Desmorat [2010]. We assume the following evolution equations for the kinematic variables.

$$\dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}^{in}_{k_\alpha(i)} - \overline{d}_i(\overline{\boldsymbol{X}}, \boldsymbol{\alpha}, \boldsymbol{\lambda}, \theta, \boldsymbol{\sigma}), \qquad i \in \{1, \ldots, N_\alpha\}. \tag{3.75}$$

Now, the $\overline{\boldsymbol{d}}_i$ are given *matrix* functions depending on the quoted quantities and possibly on further ones like accumulations. Again, the notations $\overline{\boldsymbol{X}}$, $\boldsymbol{\alpha}$ and $\boldsymbol{\lambda}$ stand for the sets of all $\boldsymbol{X}_i$, $\boldsymbol{\alpha}_i$ and λ_k, respectively. Appropriate conditions on the matrix functions $\overline{\boldsymbol{d}}_i$ ensure thermodynamic consistency. This will be considered in Subsection 3.6.

Again, in case of plastic behavior, the following restriction ensures that the evolution of $\boldsymbol{\alpha}_i$ can only take place, if the corresponding flow criterion is fulfilled. This can be expressed by

$$\lambda_{\tilde{k}_\alpha(i)} = 0 \qquad \Rightarrow \qquad \overline{\boldsymbol{d}}_i = 0 \qquad i = 1, \ldots, N_\alpha. \tag{3.76}$$

Using (3.75) and the definition of the back stresses $\overline{\boldsymbol{X}}_i$ in (3.8), general evolution equations for $\overline{\boldsymbol{X}}_i$ follow.

$$\dot{\overline{\boldsymbol{X}}}_i = \frac{2}{3} \sum_{j=1}^{N_\alpha} c_{ij} \lambda_{k_\alpha(j)} - \frac{2}{3} \sum_{j=1}^{N_\alpha} c_{ij} \overline{\boldsymbol{d}}_j(\overline{\boldsymbol{X}}, \boldsymbol{\alpha}, \boldsymbol{\lambda}, \theta, \boldsymbol{\sigma}) + \frac{2}{3} \dot{\theta} \sum_{j=1}^{N_\alpha} \frac{\mathrm{d}c_{ij}}{\mathrm{d}\theta} \boldsymbol{\alpha}_j \qquad i = 1, \ldots, N_\alpha. \tag{3.77}$$

As above, in the *regular* case $\det(\boldsymbol{c}) \neq 0$, $\boldsymbol{c}$ is invertible, and the equations (3.77) can be re-formulated without $\boldsymbol{\alpha}_j$. For a *constant* matrix $\boldsymbol{c}$, the equations (3.77) do not contain the last sum with $\boldsymbol{\alpha}_j$. Finally, from (3.9) one gets the equations for the back stresses $\boldsymbol{X}_k$ associated with the mechanisms.

$$\dot{\boldsymbol{X}}_k = \sum_{i \in \mathrm{set}_\alpha(k)} \dot{\overline{\boldsymbol{X}}}_i \qquad k = 1, \ldots, N_\alpha. \tag{3.78}$$

And, in short (cf. (3.10)) one has

$$\dot{\boldsymbol{X}} = \mathbb{C}^\alpha \dot{\overline{\boldsymbol{X}}}. \tag{3.79}$$

In many applications, the kinematic hardening is more in the focus than the isotropic one. Therefore, a great variety of proposals is in use. Thus, for a better readability we will deal separately later on with special cases of the general approach in (3.75).

Remark 3.6. Similar quite general evolution equations for the kinematic variables as in (3.60) can be found in Desmorat [2010]. There, the aim is to model hardening without saturation. This is not in the focus here.

3.6 General form of the Clausius-Planck inequality

At this stage, we present the general form of the Clausius-Planck inequality (2.22) using the information already given above. Later on, this inequality will be applied to important special cases of evolution laws for internal variables.

Based on (2.23), (2.26), (3.1), (3.7), (3.8), (3.9), (3.29), and (3.32), the Clausius-Planck inequality (2.22) becomes

$$\sum_{k=1}^{n_M} \left(\boldsymbol{\sigma}_k - \boldsymbol{X}_k \right) : \dot{\boldsymbol{\varepsilon}}^{in}_k + \sum_{i=1}^{N_\alpha} \overline{\boldsymbol{X}}_i : \left(\dot{\boldsymbol{\varepsilon}}^{in}_{k_\alpha(i)} - \dot{\boldsymbol{\alpha}}_i \right) - \sum_{i=1}^{N_q} \overline{R}_i \dot{q}_i \geq 0. \tag{3.80}$$

Moreover, using (3.33), (3.35), (3.36), (3.40), (3.49), (3.53) and (3.54) this inequality turns to

$$(3.81) \qquad \sum_{i=1}^{n_C} R_{0i}\lambda_i + \sum_{i=1}^{N_q} \overline{R}_i\big(\lambda_{k_q(i)} - \dot{q}_i\big) + \sum_{i=1}^{N_\alpha} \overline{X}_i : \Big(\dot{\varepsilon}_{k_\alpha(i)}^{in} - \dot{\alpha}_i\Big) \geq 0.$$

Assuming the evolution laws (3.60) and (3.75), the last inequality turns to

$$(3.82) \qquad \sum_{i=1}^{n_C} R_{0i}\lambda_i + \sum_{i=1}^{N_q} \overline{R}_i\overline{b}_i + \sum_{i=1}^{N_\alpha} \overline{X}_i : \overline{d}_i \geq 0.$$

Due to (3.42) and (3.54), the first sum in (3.82) is always non-negative. Hence, for thermodynamic consistency of the model under consideration the following conditions are sufficient.

$$(3.83) \qquad \sum_{i=1}^{N_q} \overline{R}_i\,\overline{b}_i(\boldsymbol{R},\boldsymbol{q},\boldsymbol{\lambda},\theta,\boldsymbol{\sigma}) \geq 0 \qquad\qquad \text{for all admissible arguments,}$$

$$(3.84) \qquad \sum_{i=1}^{N_\alpha} \overline{X}_i : \overline{d}_i(\boldsymbol{X},\boldsymbol{\alpha},\boldsymbol{\lambda},\theta,\boldsymbol{\sigma}) \geq 0 \qquad\qquad \text{for all admissible arguments,}$$

Obviously, in the special case (3.65), the positive semi-definiteness of the matrix $\boldsymbol{b}$ (for all admissible arguments) ensures the inequality (3.83).

3.7 More special evolution equations for the kinematic variables

Now, it is the aim to present some more concrete proposals being special cases of the quite general approach in (3.75). For technical reason we need a further function $\tilde{k}_\alpha : \{1,\ldots,N_\alpha\} \to \{1,\ldots,n_C\}$ attaching the number i of the variable $\boldsymbol{\alpha}_i$ to the number k of the flow criterion which contents the "home" mechanism of $\boldsymbol{\alpha}_i$. Hence, we define

$$(3.85) \qquad \tilde{k}_\alpha(i) := k_f(k_\alpha(i)) \qquad \text{for } i = 1,\ldots,N_\alpha.$$

With the help of the matrix-based presentations developed above, the use of the functions $\tilde{k}_\alpha$ can be avoided. We will do so later on. However, for a better understanding, we use $\tilde{k}_\alpha$ when introducing the approaches.

The following proposal acts on a suggestion by Burlet and Cailletaud [1987] (see Remark 3.7). The original idea was to take projections of back stresses onto the unit tensors $\boldsymbol{m}_i$ (defined in (3.52)) into account.

$$(3.86) \quad \dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}_{k_\alpha(i)}^{in} - \frac{3}{2}\sum_{j=1}^{N_\alpha} d_{ij}^{(x)} \left\{ (1-\eta_{ij}^{(x)})\,\overline{X}_j + \eta_{ij}^{(x)}(\overline{X}_j : \boldsymbol{m}_{k_\alpha(j)})\,\boldsymbol{m}_{k_\alpha(i)} \right\} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}\,\sqrt{\lambda_{\tilde{k}_\alpha(j)}} +$$

$$-\sum_{j=1}^{N_\alpha} d_{ij}^{(\alpha)} \left\{ (1-\eta_{ij}^{(\alpha)})\,\boldsymbol{\alpha}_j + \eta_{ij}^{(\alpha)}(\boldsymbol{\alpha}_j : \boldsymbol{m}_{k_\alpha(j)})\,\boldsymbol{m}_{k_\alpha(i)} \right\} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}\,\sqrt{\lambda_{\tilde{k}_\alpha(j)}},$$

$$i \in \{1,\ldots,N_\alpha\}.$$

The matrices $\boldsymbol{d}^{(x)}$, $\boldsymbol{d}^{(\alpha)}$, $\boldsymbol{\eta}^{(x)}$ and $\boldsymbol{\eta}^{(\alpha)}$ of material parameters are *not necessarily symmetric*. In most applications one requires

$$(3.87) \qquad 0 \leq \eta_{ij}^{(x)} \leq 1, \qquad\qquad 0 \leq \eta_{ij}^{(\alpha)} \leq 1 \qquad\qquad \forall\, i,j \in \{1,\ldots,N_\alpha\}.$$

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Besides, in many applications, scalar parameters $\eta^{(x)}$, $\eta^{(\alpha)}$ are in use. As we will see in Subsection 4.1, in case on *uniaxial stress history*, these parameters drop out. This corresponds to the case $\boldsymbol{\eta} = 0$ and (3.86) turns to

$$(3.88) \qquad \dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}^{in}_{k_\alpha(i)} - \sum_{j=1}^{N_\alpha} \left(\frac{3}{2} d^{(x)}_{ij} \overline{\boldsymbol{X}}_j + d^{(\alpha)}_{ij} \boldsymbol{\alpha}_j \right) \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}, \qquad i \in \{1, \ldots, N_\alpha\}.$$

Note that the factor $^3/_2$ does not occur in front of the kinematic variables in (3.86) and (3.88). The reason for this is to get an equivalence between the $3d$ formulas and their $1d$ counterparts. We return to this matter in Subsection 4.1.

We write down the Armstrong-Frederick relations for the back stresses $\overline{\boldsymbol{X}}_i$ in case of the evolution equations (3.88).

$$(3.89) \quad \dot{\overline{\boldsymbol{X}}}_i = \frac{2}{3} \sum_{j=1}^{N_\alpha} c_{ij} \dot{\boldsymbol{\varepsilon}}^{in}_{k_\alpha(j)} - \sum_{j,s=1}^{N_\alpha} c_{ij} \left(d^{(x)}_{js} \overline{\boldsymbol{X}}_s + \frac{2}{3} d^{(\alpha)}_{js} \boldsymbol{\alpha}_s \right) \sqrt{\lambda_{\tilde{k}_\alpha(s)}} \sqrt{\lambda_{\tilde{k}_\alpha(j)}} +$$

$$+ \frac{2}{3} \dot{\theta} \sum_{j=1}^{N_\alpha} \frac{\mathrm{d}c_{ij}}{\mathrm{d}\theta} \boldsymbol{\alpha}_j \qquad i = 1, \ldots, N_\alpha.$$

Clearly, for a *constant* matrix $\boldsymbol{c}$ the equations (3.89) do not contain explicitly the kinematic variables $\boldsymbol{\alpha}_j$. In the *regular case* of a positive definite matrix $\boldsymbol{c}$, there exists the inverse matrix $\boldsymbol{c}^{-1}$. Hence, the kinematic variables can be expressed by the back stresses, and the equations (3.89) may be re-written without $\boldsymbol{\alpha}_j$. We refer to Wolff et al. [2010], Wolff et al. [2011b] for more explanation. Finally, using the definition (3.9) of the back stresses $\boldsymbol{X}_i$ associated with the ith mechanism, one has

$$(3.90) \qquad \dot{\boldsymbol{X}}_k = \sum_{i \in \mathrm{set}_\alpha(k)} \dot{\overline{\boldsymbol{X}}}_i \qquad k = 1, \ldots, n_M$$

In the *case of 1C models*, there is only one plastic multiplier λ. Hence, in (3.86), one has

$$(3.91) \qquad \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} = \lambda \qquad \forall i, j \in \{1, \ldots, N_\alpha\}.$$

In order to re-formulate the evolution equations (3.88) for $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_{N_\alpha})$ and (3.89) for the back stresses, we define a further special diagonal matrix (cf. (3.67), (3.67)).

$$(3.92) \qquad \Lambda^{(\alpha)} \in \mathbb{R}^{N_\alpha \times N_\alpha}, \qquad (\Lambda^{(\alpha)})_{ij} := diag\{(\mathbb{C}^\alpha)^T (\mathbb{C}^f)^T \sqrt{\lambda}\}$$

Moreover, we need a special version of the partial plastic strains defined by

$$(3.93) \qquad \overline{\boldsymbol{\varepsilon}}^{in}_{(m)} := \left(\mathbb{C}^\alpha \right)^T \boldsymbol{\varepsilon}^{in}_{(m)}.$$

Finally, we can re-formulate the evolutions equation (3.88) for $\boldsymbol{\alpha}$ as well as the evolution equations (3.89) and (3.90) for $\overline{\boldsymbol{X}}$ and $\boldsymbol{X}$, respectively.

$$(3.94) \qquad \dot{\boldsymbol{\alpha}} = \dot{\overline{\boldsymbol{\varepsilon}}}^{in}_{(m)} - \Lambda^{(\alpha)} \left(\frac{3}{2} \boldsymbol{d}^{(x)} \Lambda^{(\alpha)} \overline{\boldsymbol{X}} + \boldsymbol{d}^{(\alpha)} \Lambda^{(\alpha)} \boldsymbol{\alpha} \right),$$

$$(3.95) \qquad \dot{\overline{\boldsymbol{X}}} = \boldsymbol{c} \left(\dot{\overline{\boldsymbol{\varepsilon}}}^{in}_{(m)} - \Lambda^{(\alpha)} \left(\frac{3}{2} \boldsymbol{d}^{(x)} \Lambda^{(\alpha)} \overline{\boldsymbol{X}} + \boldsymbol{d}^{(\alpha)} \Lambda^{(\alpha)} \boldsymbol{\alpha} \right) \right) + \dot{\theta} \left(\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}\theta} \right) \boldsymbol{\alpha},$$

$$(3.96) \qquad \dot{\boldsymbol{X}} = \mathbb{C}^\alpha \dot{\overline{\boldsymbol{X}}}.$$

The case with the Burlet-Cailletaud approach (3.86) can be dealt with in an analogous manner. We drop this here because of only dealing with uniaxial experiments in the forthcoming simulations.

The quite general approach (3.86) includes used variants as well as new ones. We present *three important special cases*. Clearly, for these special cases the Armstrong-frederick relations can be written down in an analogous manner as in (3.89). We drop this here.

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3.7.1 Case of MM models with only one kinematic variable α per mechanism

For each mechanism $k \in \{1, \ldots, n_M\}$ there holds $N_\alpha^{(k)} = 1$. Thus, in (3.86), one has $k_\alpha(i) = i$ for all $i = 1, \ldots, n_M$. In other words, in this case the structural matrix $\mathbb{C}$ is the $n_M \times n_M$ identity matrix, and $\overline{\varepsilon}_{(m)}^{in}$ equals to $\varepsilon_{(m)}^{in}$ (cf. (3.93)). Thus, the approach (3.86) will be simplified to

$$(3.97) \quad \dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}_i^{in} - \frac{3}{2} \sum_{j=1}^{n_M} d_{ij}^{(x)} \left\{ (1 - \eta_{ij}^{(x)}) \, \overline{\boldsymbol{X}}_j + \eta_{ij}^{(x)} (\overline{\boldsymbol{X}}_j : \boldsymbol{m}_j) \, \boldsymbol{m}_i \right\} \sqrt{\lambda_{k_f(i)}} \sqrt{\lambda_{k_f(j)}} +$$

$$- \sum_{j=1}^{n_M} d_{ij}^{(\alpha)} \left\{ (1 - \eta_{ij}^{(\alpha)}) \, \boldsymbol{\alpha}_j + \eta_{ij}^{(\alpha)} (\boldsymbol{\alpha}_j : \boldsymbol{m}_j) \, \boldsymbol{m}_i \right\} \sqrt{\lambda_{k_f(j)}} \sqrt{\lambda_{k_f(i)}} \qquad i \in \{1, \ldots, n_M\}.$$

This variant of n_M models has been usually applied with *diagonal* matrices $\boldsymbol{d}$ (i.e., $d_{ij} = 0$, if $i \neq j$). The general case with not necessarily symmetric matrices $\boldsymbol{d}$ has been proposed in Wolff et al. [2011b]. More comments are given in Remark 3.8 (ii).

Further specialization occur, if only the proper projections $(\boldsymbol{X}_j : \boldsymbol{m}_j) \, \boldsymbol{m}_j$ will be taken into account. This can be achieved by setting $\eta_{ij} := 0$ for $i \neq j$. Analogously, the terms with $\boldsymbol{\alpha}_j$ can be dealt with.

3.7.2 Case of 1M models with r kinematic variables α ("Chaboche models")

Now one has $n_M = 1$, $N_\alpha^{(1)} = r$, and the structural matrix $\mathbb{C}$ consists of one row with length $N_\alpha^{(1)} = r$ completely fulfilled by one. Thus, the approach (3.86) simplifies to (with ε_{in} instead of ε_1, and with $\boldsymbol{m}$ instead of $\boldsymbol{m}_1$)

$$(3.98) \qquad \dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}_{in} - \frac{3}{2} \sum_{j=1}^{r} d_{ij}^{(x)} \left\{ (1 - \eta_{ij}^{(x)}) \, \overline{\boldsymbol{X}}_j + \eta_{ij}^{(x)} (\overline{\boldsymbol{X}}_j : \boldsymbol{m}) \, \boldsymbol{m} \right\} \lambda +$$

$$- \sum_{j=1}^{r} d_{ij}^{(\alpha)} \left\{ (1 - \eta_{ij}^{(\alpha)}) \, \boldsymbol{\alpha}_j + \eta_{ij}^{(\alpha)} (\boldsymbol{\alpha}_j : \boldsymbol{m}) \, \boldsymbol{m} \right\} \lambda \qquad i = 1, \ldots, r.$$

Formally, one has $\overline{\varepsilon}_{(m)}^{in} = \varepsilon^{in} \, \boldsymbol{I}_{r \times r}$ with the $r \times r$ identity matrix. This approach is typical for "Chaboche models" and it covers many of their variants (see Bari and Hassan [2002], Abdel-Karim [2009a], Abdel-Karim [2010], e.g.).

3.7.3 Case of MM models with coupling only inside the mechanisms

The n_M mechanisms of a given n_M model may have more than one kinematic variable $\boldsymbol{\alpha}$, but the coupling in their evolution equations takes only place *inside* of the corresponding mechanism. That means, the approach (3.86) will be specialized in the following way.

$$(3.99) \qquad \dot{\boldsymbol{\alpha}}_i = \dot{\boldsymbol{\varepsilon}}_{k_\alpha(i)}^{in} +$$

$$- \frac{3}{2} \sum_{j \in \mathrm{set}(k_\alpha(i))} d_{ij}^{(x)} \left\{ (1 - \eta_{ij}^{(x)}) \, \overline{\boldsymbol{X}}_j + \eta_{ij}^{(x)} (\overline{\boldsymbol{X}}_j : \boldsymbol{m}_{k_\alpha(i)}) \, \boldsymbol{m}_{k_\alpha(i)} \right\} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} \sqrt{\lambda_{\tilde{k}_\alpha(j)}} +$$

$$- \sum_{j \in \mathrm{set}(k_\alpha(i))} d_{ij}^{(\alpha)} \left\{ (1 - \eta_{ij}^{(\alpha)}) \, \boldsymbol{\alpha}_j + \eta_{ij}^{(\alpha)} (\boldsymbol{\alpha}_j : \boldsymbol{m}_{k_\alpha(i)}) \, \boldsymbol{m}_{k_\alpha(i)} \right\} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} \sqrt{\lambda_{\tilde{k}_\alpha(j)}}$$

$$i \in \{1, \ldots, N_\alpha\}.$$

In other words, in the evolution equation of $\boldsymbol{\alpha}_i$, there occur only $\overline{\boldsymbol{X}}_j$, $\boldsymbol{\alpha}_j$ and $\boldsymbol{m}_j$ belonging to the *same* mechanism as $\boldsymbol{\alpha}_i$. Formally, the variant (3.99) follows from the general one (3.86) by setting $d_{ij}^{(x)} := 0$ for $j \notin \mathrm{set}(k_\alpha(i))$.

We conclude this subsection with several remarks.

Remark 3.7. (Burlet-Cailletaud approach) The original idea of the projection of $\overline{\boldsymbol{X}}_j$ onto $\boldsymbol{m}_j$ is due to Burlet and Cailletaud [1987] (there with $\eta = 1$). The modification with a (scalar) $0 \le \eta \le 1$ was used in Taleb et al. [2006]. The aim of theses proposals was to get a better description of *bi-axial* ratcheting behavior. As we will see in Subsection 4.1, in case of *uniaxial stress history*, this approach does not play any role. The brackets in (3.88) will be simply re-placed by $\overline{\boldsymbol{X}}_j$ and by $\boldsymbol{\alpha}_j$, respectively. That means, one has

$$(3.100) \qquad \left\{ (1 - \eta_{ij}^{(x)}) \overline{\boldsymbol{X}}_j + \eta_{ij}^{(x)} (\overline{\boldsymbol{X}}_j : \boldsymbol{m}_l) \, \boldsymbol{m}_l \right\} = \boldsymbol{X}_j \quad \forall \, i, j, l$$

and an analogous result concerning the $\boldsymbol{\alpha}$ term. Thus, for applications to uniaxial experiments this approach does not play any role. Hence, the parameters η_i *cannot* be determined by uniaxial experiments.

Remarks 3.8. (i) In many applications, one encounters the approach (3.88) *either* only with back stresses *or* only with kinematic variables. In some earlier publications, 2M models with $\boldsymbol{d}^{(\alpha)} = 0$ have been called 2M-a models, and 2M models with $\boldsymbol{d}^{(x)} = 0$ have been called 2M-b models. See Wolff and Taleb [2008], Wolff et al. [2010], Wolff et al. [2011b].
At first, the approach (3.88) with $\boldsymbol{d}^{(x)} = 0$ has been proposed in Taleb et al. [2006] for a better description of ratcheting behavior.

(ii) Usually, *diagonal* matrices $\boldsymbol{d}^{(x)}$ and $\boldsymbol{d}^{(\alpha)}$ have been used. The generalization to not necessarily symmetric matrices has been proposed in Wolff et al. [2011b] and leads to generally *non-symmetric* generalized Armstrong-Frederick relations for the back stresses $\boldsymbol{X}_j$.

(iii) Using (3.8), the back stresses can be substituted by the kinematic variables, and, without any loss of generality the approach (3.88) can be applied with $\boldsymbol{d}^{(x)} = 0$. Nevertheless, since many approaches in use have the form (3.88) with $\boldsymbol{d}^{(\alpha)} = 0$, here, we do not proceed in this way.

(iv) If the matrix $\boldsymbol{c}$ is positive definite (for all admissible temperatures) (see Remark 3.2 (iii)), than it is invertible, and the $\boldsymbol{\alpha}_i$ can be expressed by the back stresses via (3.8). Thus, in this *regular case*, one can assume that in (3.88) only the back stresses occur.

(v) In principle, instead of the scalar parameters c_{ij} and d_{ij} material tensors E_{ij} and D_{ij} of fourth order could be used ($i, j = 1, 2$). This approach has been used in Wolff et al. [2012a] with respect to 2M models with visco-elastic mechanisms.

3.8 Clausius-Planck inequality and thermodynamic consistency for some special cases

Taking the evolution equations (3.65) and (3.88) for q_i and $\boldsymbol{\alpha}_i$, respectively, into account, one gets from (3.81)

$$(3.101) \qquad \sum_{i=1}^{n_C} R_{0i} \lambda_i + \sum_{i,j=1}^{N_q} b_{ij} \overline{R}_i \overline{R}_j \sqrt{\lambda_{k_q(j)}} \sqrt{\lambda_{k_q(i)}} + \frac{3}{2} \sum_{i,j=1}^{N_\alpha} d_{ij}^{(x)} \overline{\boldsymbol{X}}_i : \overline{\boldsymbol{X}}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} +$$

$$+ \sum_{i,j=1}^{N_\alpha} d_{ij}^{(\alpha)} \overline{\boldsymbol{X}}_i : \boldsymbol{\alpha}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} \ge 0.$$

Expressing the back stresses $\overline{\boldsymbol{X}}_i$ by the variables $\boldsymbol{\alpha}_j$ via (3.8), the inequality (3.101) becomes

$$(3.102) \quad \sum_{i=1}^{n_C} R_{0i}\lambda_i + \sum_{i,j=1}^{N_q} b_{ij}\overline{R}_i\overline{R}_j \sqrt{\lambda_{k_q(j)}} \sqrt{\lambda_{k_q(i)}} + \frac{3}{2} \sum_{i,j=1}^{N_\alpha} d_{ij}^{(x)}\overline{\boldsymbol{X}}_i : \overline{\boldsymbol{X}}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}+$$

$$+ \frac{2}{3} \sum_{i,j=1}^{N_\alpha} \sum_{s=1}^{N_\alpha} d_{ij}^{(\alpha)}c_{is}\boldsymbol{\alpha}_s : \boldsymbol{\alpha}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} \geq 0.$$

This inequality is true, if the matrices $\boldsymbol{b}$ and $\boldsymbol{d}^{(x)}$ are positive semi-definite, and if $\boldsymbol{d}^{(\alpha)}$ fulfils the following conditions.

$$(3.103) \quad \sum_{i,j,s=1}^{N_\alpha} d_{ij}^{(\alpha)}c_{is} \xi_{sj} \zeta_j \zeta_i \geq 0, \qquad \forall \xi \in \mathbb{R}^{N_\alpha^2} \qquad \forall \zeta \in \mathbb{R}^{N_\alpha}.$$

Note that the matrix $\boldsymbol{c}$ is involved in (3.103). In the case of 1C models, there is only one λ. Hence, the positive semi-definiteness of $\boldsymbol{b}$, $\boldsymbol{d}^{(x)}$ and $\boldsymbol{c}^T\boldsymbol{d}^{(\alpha)}$ ensures thermodynamic consistency. Here, $\boldsymbol{c}^T$ is the transposed matrix of $\boldsymbol{c}$.

In the case (3.86) the inequality (3.101) becomes

$$(3.104) \quad \sum_{i=1}^{n_C} R_{0i}\lambda_i + \sum_{i,j=1}^{N_q} b_{ij}\overline{R}_i\overline{R}_j \sqrt{\lambda_{k_q(j)}} \sqrt{\lambda_{k_q(i)}}+$$

$$+ \frac{3}{2} \sum_{i,j=1}^{N_\alpha} d_{ij}^{(x)}(1 - \eta_{ij}^{(x)})\overline{\boldsymbol{X}}_i : \overline{\boldsymbol{X}}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}+$$

$$+ \frac{2}{3} \sum_{i,j=1}^{N_\alpha} \sum_{s=1}^{N_\alpha} d_{ij}^{(\alpha)}(1 - \eta_{ij}^{(\alpha)})c_{is}\boldsymbol{\alpha}_s : \boldsymbol{\alpha}_j \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}+$$

$$+ \frac{3}{2} \sum_{i,j=1}^{N_\alpha} d_{ij}^{(x)}\eta_{ij}^{(x)}(\overline{\boldsymbol{X}}_j : \boldsymbol{m}_{k_\alpha(j)})(\overline{\boldsymbol{X}}_i : \boldsymbol{m}_{k_\alpha(i)}) \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}}+$$

$$+ \frac{2}{3} \sum_{i,j=1}^{N_\alpha} \sum_{s=1}^{N_\alpha} d_{ij}^{(\alpha)}\eta_{ij}^{(\alpha)}c_{is}(\boldsymbol{\alpha}_j : \boldsymbol{m}_{k_\alpha(j)})(\boldsymbol{\alpha}_s : \boldsymbol{m}_{k_\alpha(i)}) \sqrt{\lambda_{\tilde{k}_\alpha(j)}} \sqrt{\lambda_{\tilde{k}_\alpha(i)}} \geq 0.$$

To ensure this inequality, suitable semi-definiteness conditions involving the matrices $\boldsymbol{d}^{(x)}$, $\boldsymbol{d}^{(\alpha)}$, $\boldsymbol{c}$, $\boldsymbol{\eta}^{(\alpha)}$, and $\boldsymbol{\eta}^{(x)}$ must be fulfilled (besides the positive semi-definiteness of $\boldsymbol{b}$).

3.9 Applications of the new items to the reference model

In order to illustrate the quite general cases above, now we consider some corresponding cases for the reference 2M model presented in Subsection 3.1.3. This model is characterized by its structural matrix $\mathbb{C}^\alpha$ (cf. (3.16))

$$(3.105) \quad \mathbb{C}^\alpha = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

That means, the first mechanism has two internal kinematic variables $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$, and the second mechanism has the single kinematic variable $\boldsymbol{\alpha}_3$, in short:

$$(3.106) \quad n_M = 2, \qquad N_\alpha^{(1)} = 2, \qquad N_\alpha^{(2)} = 1, \qquad N_\alpha = 3.$$

Moreover, the 2M model under consideration is characterized by the symmetric 3×3 parameter matrix given in (3.16). Therefore, the (partial) back stresses $\overline{\boldsymbol{X}}_i$ ($i = 1, 2, 3$) are defined by (3.17), and the back stresses $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ associated with the mechanisms 1 and 2 are defined by (3.18). For a better readability we repeat them.

$$(3.107) \qquad \overline{\boldsymbol{X}}_1 = \frac{2}{3} \sum_{j=1}^{3} c_{1j} \boldsymbol{\alpha}_j, \qquad \overline{\boldsymbol{X}}_2 = \frac{2}{3} \sum_{j=1}^{3} c_{2j} \boldsymbol{\alpha}_j, \qquad \overline{\boldsymbol{X}}_3 = \frac{2}{3} \sum_{j=1}^{3} c_{3j} \boldsymbol{\alpha}_j,$$

$$(3.108) \qquad \boldsymbol{X}_1 = \overline{\boldsymbol{X}}_1 + \overline{\boldsymbol{X}}_2, \qquad \boldsymbol{X}_2 = \overline{\boldsymbol{X}}_3, \qquad\qquad .$$

Due to symmetry, the matrix $\boldsymbol{c}$ has six coefficients which are material parameters.

3.9.1 Two-criteria model

At first, we assume that our reference 2M model has two criteria, and that the first criterion has two isotropic internal variables q_1, q_2, and that the second criterion has one isotropic variable q_3. In a 2M2C model, each mechanism has its own criterion. Thus, the structural matrices $\mathbb{C}^f$ and $\mathbb{C}^q$ are given by

$$(3.109) \qquad \mathbb{C}^f = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathbb{C}^q = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

And, there hold

$$(3.110) \qquad n_C = 2, \qquad N_q^{(1)} = 2, \qquad N_q^{(2)} = 1, \qquad N_q = 3.$$
$$(3.111) \qquad N_f^{(1)} = 1, \qquad N_f^{(2)} = 1.$$

Thus, we have three (partial) isotropic hardening stresses $\overline{R}_i$ ($i = 1, 2, 3$) and two isotropic hardening stresses R_1, R_2 associated with the first and second criterion, respectively. Summarizing, there hold the following relations.

$$(3.112) \qquad \overline{R}_i = \sum_{j=1}^{3} Q_{ij} \, q_j, \qquad\qquad i = 1, 2, 3.$$
$$(3.113) \qquad R_1 = \overline{R}_1 + \overline{R}_2, \qquad\qquad R_2 = \overline{R}_3.$$

Due to symmetry, the matrix $\boldsymbol{Q}$ has six coefficients. Clearly, we have to plastic multipliers λ_1 and λ_2 associated with the first and second criterion, respectively.

Now, the general approach in (3.88) yields in our concrete case.

$$(3.114) \qquad \dot{\boldsymbol{\alpha}}_1 = \dot{\boldsymbol{\varepsilon}}_1^{in} - \sum_{j=1}^{2} \left\{ \frac{3}{2} d_{1j}^{(x)} \overline{\boldsymbol{X}}_j + d_{1j}^{(\alpha)} \boldsymbol{\alpha}_j \right\} \lambda_1 - \left\{ \frac{3}{2} d_{13}^{(x)} \overline{\boldsymbol{X}}_3 + d_{13}^{(\alpha)} \boldsymbol{\alpha}_3 \right\} \sqrt{\lambda_1} \sqrt{\lambda_2},$$

$$(3.115) \qquad \dot{\boldsymbol{\alpha}}_2 = \dot{\boldsymbol{\varepsilon}}_1^{in} - \sum_{j=1}^{2} \left\{ \frac{3}{2} d_{2j}^{(x)} \overline{\boldsymbol{X}}_j + d_{2j}^{(\alpha)} \boldsymbol{\alpha}_j \right\} \lambda_1 - \left\{ \frac{3}{2} d_{23}^{(x)} \overline{\boldsymbol{X}}_3 + d_{23}^{(\alpha)} \boldsymbol{\alpha}_3 \right\} \sqrt{\lambda_1} \sqrt{\lambda_2},$$

$$(3.116) \qquad \dot{\boldsymbol{\alpha}}_3 = \dot{\boldsymbol{\varepsilon}}_2^{in} - \sum_{j=1}^{2} \left\{ \frac{3}{2} d_{3j}^{(x)} \overline{\boldsymbol{X}}_j + d_{3j}^{(\alpha)} \boldsymbol{\alpha}_j \right\} \sqrt{\lambda_2} \sqrt{\lambda_1} - \left\{ \frac{3}{2} d_{33}^{(x)} \overline{\boldsymbol{X}}_3 + d_{33}^{(\alpha)} \boldsymbol{\alpha}_3 \right\} \lambda_2.$$

Generally, each of the matrices $\boldsymbol{d}^{(x)}$ and $\boldsymbol{d}^{(\alpha)}$ has nine coefficients being material functions. Considering special cases, this number will be reduced. For instance, if only the back stresses occur (i.e. $\boldsymbol{d}^{(\alpha)} =$

0), there remain only nine coefficients. Assuming additionally, that the coupling within the evolution equations occurs only within the mechanisms, the coefficients d_{13}, d_{23}, d_{31}, and d_{32} become zero. This yields fife non-vanishing coefficients of $\boldsymbol{d}^{(x)}$

It is possible, of course, to consider the more general case (3.86). We drop this here, focussing on processing of data stemming from uniaxial experiments (see Subsection 4.1).

The evolution equations for q_i are given by (cf. (3.65))

$$(3.117) \qquad \dot{q}_1 = \lambda_1 - b_{11}\overline{R}_1\lambda_1 - d_{12}\overline{R}_2\lambda_1 - b_{13}\overline{R}_3\sqrt{\lambda_1}\sqrt{\lambda_2},$$

$$(3.118) \qquad \dot{q}_2 = \lambda_1 - b_{21}\overline{R}_1\lambda_1 - d_{22}\overline{R}_2\lambda_1 - b_{23}\overline{R}_3\sqrt{\lambda_1}\sqrt{\lambda_2},$$

$$(3.119) \qquad \dot{q}_3 = \lambda_2 - b_{31}\overline{R}_1\sqrt{\lambda_1}\sqrt{\lambda_2} - d_{32}\overline{R}_2\sqrt{\lambda_1}\sqrt{\lambda_2} - b_{33}\overline{R}_3\lambda_2.$$

Obviously, the (not necessarily symmetric) matrix $\boldsymbol{b}$ has nine coefficients.

In accordance with (3.55), we get special vectors of plastic multipliers stemming from $\boldsymbol{\lambda} = (\lambda_1, \lambda_2)$.

$$(3.120) \qquad \boldsymbol{\lambda}^{(q)} = \boldsymbol{\lambda}^{(\alpha)} = (\lambda_1, \lambda_1, \lambda_2), \qquad\qquad \boldsymbol{\lambda}^{(m)} = \boldsymbol{\lambda} = (\lambda_1, \lambda_2).$$

Moreover, in accordance with (3.93) one has

$$(3.121) \qquad \overline{\varepsilon}^{in}_{(m)} = (\varepsilon^{in}_1, \varepsilon^{in}_1, \varepsilon^{in}_2).$$

The special diagonal matrices $\Lambda^{(q)}$ and $\Lambda^{(\alpha)}$ defined in (3.67) and (3.92), respectively, read as

$$(3.122) \qquad \Lambda^{(q)} = \Lambda^{(\alpha)} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & 0 \\ 0 & \sqrt{\lambda_1} & 0 \\ 0 & 0 & \sqrt{\lambda_2} \end{pmatrix}.$$

Using the matrices $\Lambda^{(q)}$ and $\Lambda^{(\alpha)}$ as well as $\overline{\varepsilon}^{in}_{(m)}$, the evolution equations (3.114) – (3.119) can be transformed into matrix-based relations as in (3.69) and (3.94). Finally, from (3.114) – (3.119) and from (3.66) and (3.89) the evolution equations for $\overline{R}_i$ $(i = 1, \ldots, n_C)$ and for $\overline{X}_j$ $(j = 1, \ldots, N_\alpha)$ follow.

In accordance with (3.35) and (3.36) we have the quantities

$$(3.123) \quad J_1 = \overline{J}_1 = \left(\frac{3}{2}(\boldsymbol{\sigma}^*_1 - \boldsymbol{X}^*_1) : (\boldsymbol{\sigma}^*_1 - \boldsymbol{X}^*_1)\right)^{\frac{1}{2}} \quad J_2 = \overline{J}_2 = \left(\frac{3}{2}(\boldsymbol{\sigma}^*_2 - \boldsymbol{X}^*_2) : (\boldsymbol{\sigma}^*_2 - \boldsymbol{X}^*_2)\right)^{\frac{1}{2}},$$

as well as the two yield functions f_1, f_2 (cf. (3.40)

$$(3.124) \qquad f_i(\boldsymbol{\sigma}_i, \boldsymbol{X}_i, R_i, R_{0i}) = J_i - (R_i + R_{0i}) \qquad\qquad i = 1, 2.$$

The tensors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ are defined in accordance with (3.49). Finally, the evolution of ε_1 and ε_2 is given by (3.53). In the case under consideration, due to $n_M = n_C$, one gets a simpler formula.

$$(3.125) \qquad \dot{\boldsymbol{\varepsilon}}^{in}_i = \lambda_i \frac{3}{2} \frac{\boldsymbol{\sigma}^*_i - \boldsymbol{X}^*_i}{J_i}, \qquad\qquad i = 1, 2.$$

Summarizing the considerations above, the 2M2C model has the following parameters

(3.126)	c_{ij}	$i, j \in \{1, 2, 3\}$, $i \leq j$	6 parameters,
(3.127)	$d^{(x)}_{ij}$	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.128)	$d^{(\alpha)}_{ij}$	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.129)	Q_{ij}	$i, j \in \{1, 2, 3\}$, $i \leq j$	6 parameters,
(3.130)	b_{ij}	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.131)	$A_1, A_2, \sigma_{01}, \sigma_{01}$		4 parameters.

Clearly, in special cases, the numbers will be reduced. Moreover, the Clausius-Planck inequality (3.102) reads as

$$
(3.132) \quad \sum_{i=1}^{2} R_{0i}\lambda_i + \sum_{i,j=1}^{2} b_{ij}\overline{R}_i\overline{R}_j\lambda_1 + \sum_{j=1}^{2}(b_{j3}+b_{3j})\overline{R}_3\overline{R}_j\,\sqrt{\lambda_1}\,\sqrt{\lambda_2} + b_{33}\overline{R}_3^2\lambda_2 +
$$

$$
+ \frac{3}{2}\sum_{i,j=1}^{2} d_{ij}^{(x)}\overline{\boldsymbol{X}}_i : \overline{\boldsymbol{X}}_j\lambda_1 + \frac{3}{2}\sum_{j=1}^{2}(d_{j3}^{(x)}+d_{3j}^{(x)})\overline{\boldsymbol{X}}_3 : \overline{\boldsymbol{X}}_j\sqrt{\lambda_1}\,\sqrt{\lambda_2} + \frac{3}{2}d_{33}^{(x)}\overline{\boldsymbol{X}}_3 : \overline{\boldsymbol{X}}_3\lambda_2 +
$$

$$
+ \frac{2}{3}\sum_{j=1}^{2}\sum_{s=1}^{3}\Big(\sum_{i=1}^{2} c_{si}^{T}d_{ij}^{(\alpha)}\sqrt{\lambda_1} + c_{s3}^{T}d_{3j}^{(\alpha)}\sqrt{\lambda_2}\Big)\boldsymbol{\alpha}_s : \boldsymbol{\alpha}_j\sqrt{\lambda_1} +
$$

$$
+ \frac{2}{3}\sum_{s=1}^{3}\Big(\sum_{i=1}^{2} c_{si}^{T}d_{i3}^{(\alpha)}\sqrt{\lambda_1} + c_{s3}^{T}d_{33}^{(\alpha)}\sqrt{\lambda_2}\Big)\boldsymbol{\alpha}_s : \boldsymbol{\alpha}_3\sqrt{\lambda_2} \geq 0.
$$

In accordance with the general case (see (3.102)) this inequality is fulfilled, if the matrices $\boldsymbol{b}$ and $\boldsymbol{d}^{(x)}$ are positive semi-definite and if the the matrix $\boldsymbol{d}^{(\alpha)}$ fulfills (3.103). For special cases, this condition can be simplified.

3.9.2 One-criterion model

Now, we assume that our 2M model has only one flow criterion. Thus, the structural matrix $\mathbb{C}^f$ is given by

$$
(3.133) \qquad\qquad \mathbb{C}^f = \begin{pmatrix} 1 & 1 \end{pmatrix}.
$$

The structural matrix $\mathbb{C}^\alpha$ remains as in (3.105). Furthermore, we assume three isotropic variables q_i ($i = 1, 2, 3$) associated to the single criterion. This yields the structural matrix $\mathbb{C}^q$ as

$$
(3.134) \qquad\qquad \mathbb{C}^q = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}.
$$

Therefore, the numbers connected with the flow criterion and with the isotropic variables read as

$$
(3.135) \qquad n_C = 1, \qquad N_q^{(1)} = 3, \qquad N_q = 3, \qquad N_f^{(1)} = 2.
$$

The numbers $n_M = 2$, $N_\alpha^{(1)} = 2$, $N_\alpha^{(2)} = 1$ and $N_\alpha = 3$ are the same as in (3.106). The back stresses $\overline{\boldsymbol{X}}_i$ and $\boldsymbol{X}_j$ are defined as in (3.107) and (3.108). Moreover, the isotropic hardening stresses $\overline{R}_i$ are defined as in (3.112), but, now one has

$$
(3.136) \qquad\qquad R = R_1 = \overline{R}_1 + \overline{R}_2 + \overline{R}_3.
$$

Due to symmetry, the matrix $\boldsymbol{Q}$ has six coefficients. Moreover, $\overline{J}_1$ and $\overline{J}_2$ are defined as in (3.123), and $J = J_1$ is given by

$$
(3.137) \qquad\qquad J := \left(\overline{J}_1^\beta + \overline{J}_2^\beta\right)^{\frac{1}{\beta}}
$$

with $\beta > 0$. The single flow function $f = f_1$ is defined by

$$
(3.138) \qquad\qquad f(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{X}_1, \boldsymbol{X}_2, R, R_0) := J - (R + R_0)
$$

with $R_{01} := \sqrt[\beta]{2}\,\sigma_{01}$. The evolution equations for $\boldsymbol{\alpha}_i$ are the same as in (3.114) – (3.116) only with $\lambda = \lambda_1 = \lambda_2$. Thus, a more compact notation is possible

$$(3.139) \qquad \dot{\boldsymbol{\alpha}}_1 = \dot{\boldsymbol{\varepsilon}}_1^{in} - \sum_{j=1}^{3}\left\{\frac{3}{2}d_{1j}^{(x)}\overline{\boldsymbol{X}}_j + d_{1j}^{(\alpha)}\boldsymbol{\alpha}_j\right\}\lambda,$$

$$(3.140) \qquad \dot{\boldsymbol{\alpha}}_2 = \dot{\boldsymbol{\varepsilon}}_1^{in} - \sum_{j=1}^{3}\left\{\frac{3}{2}d_{2j}^{(x)}\overline{\boldsymbol{X}}_j + d_{2j}^{(\alpha)}\boldsymbol{\alpha}_j\right\}\lambda,$$

$$(3.141) \qquad \dot{\boldsymbol{\alpha}}_3 = \dot{\boldsymbol{\varepsilon}}_2^{in} - \sum_{j=1}^{3}\left\{\frac{3}{2}d_{3j}^{(x)}\overline{\boldsymbol{X}}_j + d_{3j}^{(\alpha)}\boldsymbol{\alpha}_j\right\}\lambda.$$

Due to only one criterion, the evolution equations for q_j can be written in the following way.

$$(3.142) \qquad \dot{q}_i = \lambda - \sum_{j=1}^{3} b_{ij}\overline{R}_j\lambda.$$

Moreover, using (3.66) and (3.89), the evolution equations for $\boldsymbol{R}$ and $\boldsymbol{X}$ can be written down without difficulties.

Summarizing, the reference 2M1C model has the following material parameters:

(3.143)	c_{ij}	$i, j \in \{1, 2, 3\}$, $i \leq j$	6 parameters,
(3.144)	$d_{ij}^{(x)}$	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.145)	$d_{ij}^{(\alpha)}$	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.146)	Q_{ij}	$i, j \in \{1, 2, 3\}$, $i \leq j$	6 parameters,
(3.147)	b_{ij}	$i, j \in \{1, 2, 3\}$	9 parameters,
(3.148)	$A_1, A_2, \sigma_{01}, \beta$		4 parameters.

In both cases of the 2M models considered here, the parameters A_1 and A_2 are positive numbers, the parameters c_{ij}, Q_{ij} and σ_{0i} ($i = 1$ or $i = 1, 2$) are generally temperature-depending, the remaining parameters d_{ij}, b_{ij} and β may depend on temperature and further quantities.

In the case of the 2M1C model, the Clausius-Planck inequality (3.102) reads as

$$(3.149) \qquad R_0\lambda + \lambda\sum_{i,j=1}^{3} b_{ij}\overline{R}_i\overline{R}_j + \frac{3}{2}\lambda\sum_{i,j=1}^{3} d_{ij}^{(x)}\overline{\boldsymbol{X}}_i : \overline{\boldsymbol{X}}_j + \frac{2}{3}\lambda\sum_{i,j=1}^{3}\sum_{s=1}^{3} c_{si}^T d_{ij}^{(\alpha)}\boldsymbol{\alpha}_s : \boldsymbol{\alpha}_j \geq 0.$$

Clearly, this inequality is fulfilled, if the matrices $\boldsymbol{b}$, $\boldsymbol{d}^{(x)}$ and $\boldsymbol{c}^T\boldsymbol{d}^{(\alpha)}$ are positive semi-definite.

3.10 Summary of the model

Concluding the modeling part of this study, we summarize the general multi-mechanism model (in series) developed above.

At first, there are the impulse equation (2.1), the heat-conduction equation (2.31), the (isotropic) stress-strain relation (2.18), Fourier's law (2.20), the definition (2.4) of $\boldsymbol{\varepsilon}$ and the additive decomposition (2.8) of the total strain as well as the initial and boundary conditions (2.5) – (2.7).

This part of the model (named conditionally "thermoelastic") is governed by the following parameters and given quantities:

$$(3.150) \qquad \varrho_0, \quad \mu, \quad \lambda_L, \quad \alpha_\theta, \quad c_d, \quad \kappa_\theta, \quad \delta_\theta, \quad \theta_0, \quad \theta_\Gamma, \quad \boldsymbol{\tau}, \quad \boldsymbol{f}, \quad r.$$

The inelastic part of a multi-mechanism model is characterized by n_M mechanisms. That means, the inelastic, here plastic behavior is determined by the decomposition (2.23) of the inelastic strain ε_{in}:

$$(3.151) \qquad \varepsilon_{in} = \sum_{j=1}^{n_M} A_j \, \varepsilon_j^{in}.$$

In this work, the numbers

$$(3.152) \qquad A_j > 0 \qquad\qquad\qquad j = 1, \ldots, n_M$$

are parameters. In special cases, on can set them equal to one. Sometimes, it is useful to collect the numbers A_j in a row vector $\boldsymbol{A}$ via

$$(3.153) \qquad \boldsymbol{A} := (A_1, \ldots, A_{n_M}).$$

As a *new item*, each mechanism i with $i \in \{1, \ldots, n_M\}$ may have $N_\alpha^{(i)}$ associated kinematic variables $\boldsymbol{\alpha}_j$. Moreover, there may be $n_C \leq n_M$ flow criteria. To each criterion several mechanisms as well as several isotropic variables q_i are associated. The full information about relations between mechanisms, flow criteria as well as kinematic and isotropic variables are given with the help of three structural matrices consisting only of ones and zeros:

$$(3.154) \qquad \mathbb{C}^\alpha \in \{0,1\}^{n_M \times N_\alpha}, \qquad \mathbb{C}^f \in \{0,1\}^{n_C \times n_M}, \qquad \mathbb{C}^q \in \{0,1\}^{n_C \times N_q}.$$

The total numbers of kinematic and isotropic variables are N_α and N_q, respectively. Note that the entrees of the three structure matrices $\mathbb{C}^\alpha$, $\mathbb{C}^f$ and $\mathbb{C}^q$ are *not* material parameters.

The $n_M n_C$ model has n_C flow functions f_k ($k = 1, \ldots, n_C$) defined by (3.40) and (3.41). Thus, the origin yield stresses σ_{0k} are further material parameters, possibly depending on temperature. Moreover, there arise n_C plastic multipliers λ_k having to fulfil the conditions (3.54), or, in a compact way (3.57). The n_M plastic mechanisms ε_i^{in} fulfil the following evolution equations.

$$(3.155) \qquad \dot{\boldsymbol{\varepsilon}}_i^{in} = \lambda_k \, \boldsymbol{n}_i, \qquad\qquad k = 1, \ldots, n_C, \qquad\qquad i \in \mathrm{set}_f(k).$$

The kinematic as well as the isotropic hardening is given by the $N_\alpha \times N_\alpha$ matrix $\boldsymbol{c}$ of generalized kinematic hardening moduli and by the $N_q \times N_q$ matrix $\boldsymbol{b}$ of generalized isotropic hardening moduli, respectively. These two matrices consists of material parameters (possibly temperature-dependent) must be symmetric and positive semi-definite. Due to the application in $1d$ simulations in this study, here we do not repeat the general approach due to Burlet-Cailletaud (3.86).

The evolution equations for the kinematic and isotropic variables (3.65) (or (3.69) in compact form) and (3.65) (or (3.94) in compact form), respectively, read as

$$(3.156) \qquad \dot{\boldsymbol{\alpha}} = (\mathbb{C}^\alpha)^T \dot{\boldsymbol{\varepsilon}}_{(m)}^{in} - \Lambda^{(\alpha)} \Big(\frac{3}{2} \boldsymbol{d}^{(x)} \, \Lambda^{(\alpha)} \, \overline{\boldsymbol{X}} + \boldsymbol{d}^{(\alpha)} \, \Lambda^{(\alpha)} \, \boldsymbol{\alpha} \Big),$$

$$(3.157) \qquad \dot{\boldsymbol{q}} = \boldsymbol{\lambda}^{(q)} - \Lambda^{(q)} \, \boldsymbol{b} \, \Lambda^{(q)} \, \overline{R}.$$

The special diagonal matrices $\Lambda^{(\alpha)}$ and $\Lambda^{(q)}$ are defined in (3.92) and (3.67), respectively, using the vector $\boldsymbol{\lambda}$ and the structural matrices. In the evolution equations (3.156), (3.157) three parameter matrices arise:

$$(3.158) \qquad \boldsymbol{b} \in \mathbb{R}^{N_q \times N_q}, \qquad\qquad \boldsymbol{d}^{(x)} \in \mathbb{R}^{N_\alpha \times N_\alpha}, \qquad\qquad \boldsymbol{d}^{(\alpha)} \in \mathbb{R}^{N_\alpha \times N_\alpha}.$$

Generally, the entries are functions depending on temperature and further quantities. The matrices $\boldsymbol{b}$ and $\boldsymbol{d}^{(x)}$ must be positive semi-definite, the matrix $\boldsymbol{d}^{(\alpha)}$ has to fulfill the condition (3.103).

Moreover, the evolution equations of $\overline{R}$, R, $\overline{X}$ and X are given as follows.

$$(3.159) \qquad \dot{\overline{R}} = \boldsymbol{Q}\Big(\boldsymbol{\lambda}^{(q)} - \Lambda^{(q)}\,\boldsymbol{b}\,\Lambda^{(q)}\,\overline{R}\Big) + \dot{\theta}\big(\frac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}\theta}\big)\boldsymbol{q},$$

$$(3.160) \qquad \dot{R} = \mathbb{C}^q\,\dot{\overline{R}}.$$

$$(3.161) \qquad \dot{\overline{X}} = \boldsymbol{c}\left((\mathbb{C}^\alpha)^T\dot{\boldsymbol{\varepsilon}}_{(m)}^{in} - \Lambda^{(\alpha)}\Big(\frac{3}{2}\boldsymbol{d}^{(x)}\,\Lambda^{(\alpha)}\,\overline{X} + \boldsymbol{d}^{(\alpha)}\,\Lambda^{(\alpha)}\,\boldsymbol{\alpha}\Big)\right) + \dot{\theta}\big(\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}\theta}\big)\boldsymbol{\alpha},$$

$$(3.162) \qquad \dot{\boldsymbol{X}} = \mathbb{C}^\alpha\,\dot{\overline{X}}.$$

4 Algorithms for simulations and parameter identification based on uniaxial experiments

We want to develop a general approach for simulations of (spatially homogenous) uniaxial material behavior as well as for determining material parameters using data obtained in uniaxial experiments. Here we focus on material behavior modeled by a multi-mechanism approach with plastic mechanisms. In Wolff et al. [2012b], an analogous approach has been developed for inelastic behavior *without* yield stress like creep and transformation-induced plasticity in steels (TRIP) (in case of one-mechanism models). Due to the general coupling within the mechanisms and to the occurrence of plastic multipliers one encounters a higher complexity. For a better readability we repeat some general items also described in Wolff et al. [2012b].

Only in simple situations, material parameters can be determined directly from experimental data as, for instance, the Young's modulus. As usual, in complex situations, before identification of parameters ("inverse problem") one has to deal with the forward problem ("direct problem") of material behavior assuming material laws and parameters to be given. Here, we only deal with discretized problems as well as with the uniaxial setting. For further discussion of general aspects of parameter identification we refer to Mahnken and Stein [1996], to Mahnken [2004] and to the references therein. For parameter identification in mechanics using $3d$ simulations we refer exemplarily to Grédiac and Pierron [2006], Avril and Pierron [2007], Lecompte et al. [2007], Cooreman et al. [2007], Kajberg and Wikman [2007], Yun and Shang [2011]. In Wolff and Böhm [2013], mathematical results for the inverse problem of parameter identification have been obtained for the case of stationary linear fully non-isotropic and non-homogeneous elasticity.

For special approaches in determining material parameters of ratcheting behavior we refer to Bari and Hassan [2000], Abdel-Karim [2005], Taleb and Cailletaud [2010], Djimli et al. [2010].

This section is arranged as follows. In Subsection 4.1, we transform the material laws used above into their "uniaxial" forms. After that, we provide formulas for postprocessing of experimental data stemming from uniaxial experiments (in Subsection 4.2). In Subsection 4.3 we develop semi-implicit algorithms for calculating the direct (discrete) problems, in a strain-driven as well as in a stress-driven version. We will use the matrix-based form developed above. Therefore, a general implementation into a matrix-processing programme package is possible, in principle for arbitrary $n_M n_C$ models. For direct calculations the programme will be given the three structural matrices (3.154), the parameter matrices $\boldsymbol{c}$, $\boldsymbol{Q}$, $\boldsymbol{b}$, $\boldsymbol{d}^{(x)}$, $\boldsymbol{d}^{(\alpha)}$ as well as the the vector $\boldsymbol{A}$ and the "thermoelastic parameters" listed up in (3.150). In Subsection 4.4 we present a scheme for parameter identification via optimization of suitable cost functionals.

4.1 Form of material laws in case of uniaxial loading

Dealing with data stemming from uniaxial experiments with small cylindrical probes, we assume spacial homogeneity and a uniaxial loading history, i.e. for all times $t \geq 0$ the stress $\boldsymbol{\sigma} = \boldsymbol{\sigma}(t)$ is directed along

the x_1 axis (i.e. the probe's axis, cf. Fig. 2). Moreover, as usual it is assumed that all inelastic strains ε_i^{in} and back stress tensors $\boldsymbol{X}_j$ are traceless:

$$(4.1) \qquad \mathrm{tr}(\varepsilon_j^{in}) = 0 \qquad j = 1, \ldots, n_M \qquad \mathrm{tr}(\overline{\boldsymbol{X}}_j) = 0 \qquad j = 1, \ldots, N_\alpha.$$

Note that (4.1) follows under mild assumptions from the evolution of internal variables (cf. Wolff et al. [2010]). Clearly, in this case, the tensorial internal variables $\boldsymbol{\alpha}_i$ are traceless, too.

Under these assumptions the following relations for the $3d$ stress tensor $\boldsymbol{\sigma}$, its deviator $\boldsymbol{\sigma}^*$, for ε_i^{in}, for $\boldsymbol{\alpha}_i$ as well as for the back stresses $\overline{\boldsymbol{X}}_i$ hold.

$$(4.2) \quad \boldsymbol{\sigma} = \begin{pmatrix} S & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \; \boldsymbol{\sigma}^* = \begin{pmatrix} \frac{2}{3}S & 0 & 0 \\ 0 & -\frac{1}{3}S & 0 \\ 0 & 0 & -\frac{1}{3}S \end{pmatrix}, \; \varepsilon_i^{in} = \begin{pmatrix} \epsilon_i^{in} & 0 & 0 \\ 0 & -\frac{1}{2}\epsilon_i^{in} & 0 \\ 0 & 0 & -\frac{1}{2}\epsilon_i^{in} \end{pmatrix},$$

$$(4.3) \qquad \overline{\boldsymbol{X}}_i = \begin{pmatrix} \overline{X}_i & 0 & 0 \\ 0 & -\frac{1}{2}\overline{X}_i & 0 \\ 0 & 0 & -\frac{1}{2}\overline{X}_i \end{pmatrix}, \; \boldsymbol{\alpha}_i = \begin{pmatrix} \alpha_i & 0 & 0 \\ 0 & -\frac{1}{2}\alpha_i & 0 \\ 0 & 0 & -\frac{1}{2}\alpha_i \end{pmatrix}, \quad i = 1, \ldots, N_\alpha.$$

Moreover, the quantities in (4.2), (4.3) are only functions of time t. Clearly, the partial stresses are given by

$$(4.4) \qquad S_i = A_i S \qquad i = 1, \ldots, n_M, \qquad\qquad \text{or} \quad \boldsymbol{S} = S\boldsymbol{A}^T.$$

Note that in this study vectors are regarded as column vectors. As an exclusion, $\boldsymbol{A}$ is regarded as a row vector.
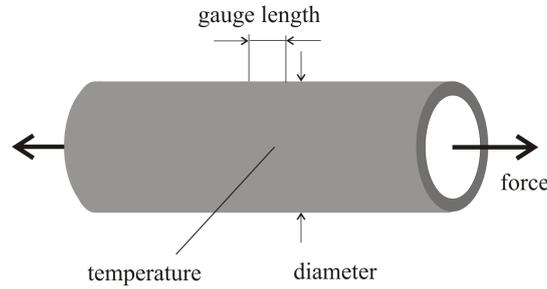
Figure 2: Scheme of a hollow probe used in servo-hydraulic testing devices. The measured data are longitudinal and transversal strains, temperature, force (and therefore stress as force per cross section) as discrete functions of time.

In (4.2), the strain in x_1-direction, ϵ_i^{in}, stands for ε_{11}^i. Here, strain tensors are denoted by ε, while *scalar strains* are denoted by ϵ. Obviously, from (2.25) and (4.2) one gets

$$(4.5) \qquad \dot{s}_i = |\dot{\epsilon}_i^{in}| \qquad i = 1, \ldots, n_M, \qquad\qquad \text{or} \quad \dot{\boldsymbol{s}} = |\dot{\boldsymbol{\epsilon}}^{in}|.$$

The last relation is understood as component-wise. We define $1d$ back stresses by

$$(4.6) \qquad \overline{x}_i := \frac{3}{2}\overline{X}_i \qquad i = 1, \ldots, N_\alpha, \qquad\qquad \text{or} \quad \overline{\boldsymbol{x}} := \frac{3}{2}\overline{\boldsymbol{X}}.$$

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The $1d$ back stresses x_i $(i = 1, \ldots, n_M)$ are defined analogously. Therefore, the *uniaxial variant* of (3.8) and (3.9) become now

$$(4.7) \qquad \overline{x}_i = \sum_{j=1}^{N_\alpha} c_{ij} \alpha_j \quad \text{for } i = 1, \ldots, N_\alpha, \qquad\qquad \text{or} \quad \overline{\boldsymbol{x}} = \boldsymbol{c} \, \boldsymbol{\alpha},$$

$$(4.8) \qquad \boldsymbol{x} = \mathbb{C}^\alpha \overline{\boldsymbol{x}}.$$

The relations for the (scalar) isotropic hardening stresses $\overline{R}_i$ (3.32) as well as for R_k in (3.33) remain unchanged.

Based on (2.26), (3.35), (4.2) and (4.3), in the uniaxial case, we have

$$(4.9) \qquad \overline{J}_i = |S_i - x_i| \quad i = 1, \ldots, n_M, \qquad\qquad \text{or} \quad \overline{\boldsymbol{J}} = |\boldsymbol{S} - \boldsymbol{x}|,$$

$$(4.10) \qquad J_k = \left(\sum_{i \in \mathrm{set}_f(k)} \overline{J}_i^{\,\beta} \right)^{\frac{1}{\beta}} \quad k = 1, \ldots, n_C, \qquad\qquad \text{or} \quad \boldsymbol{J} = \left(\mathbb{C}^f \, \overline{\boldsymbol{J}}^\beta \right)^{\frac{1}{\beta}}.$$

The yield functions f_i follow from (3.40). Now they have the following form.

$$(4.11) \qquad f_k(S_i, x_i, R_k, R_{0k}) := J_k - (R_k + R_{0k}) \qquad k = 1, \ldots, n_C, \quad i \in \mathrm{set}_f(k).$$

(The relations in (3.41) and (3.42) remain the same.) As in (3.43), we define a vector $\boldsymbol{f}^{(m)}$ of flow functions with as much as components as mechanisms.

$$(4.12) \qquad \boldsymbol{f}^{(m)} := \left(\mathbb{C}^f \right)^T \boldsymbol{f}.$$

Based on (3.49), we obtain the corresponding scalar quantities n_i as well as their compact variant.

$$(4.13) \qquad n_i = \frac{S_i - x_i}{|S_i - x_i|} \left(\frac{|S_i - x_i|}{J_k} \right)^{\beta - 1} \quad k = 1, \ldots, n_C, \quad i \in \mathrm{set}_f(k),$$

$$(4.14) \qquad \boldsymbol{n} = \frac{\boldsymbol{S} - \boldsymbol{x}}{|\boldsymbol{S} - \boldsymbol{x}|} \left(\frac{|\boldsymbol{S} - \boldsymbol{x}|}{(\mathbb{C}^f)^T \left(\mathbb{C}^f |\boldsymbol{S} - \boldsymbol{x}|^\beta \right)^{\frac{1}{\beta}}} \right)^{\beta - 1}.$$

Note that the operations in (4.14) are understood as component-wise. Now we transfer the evolution laws for ε_i^{in}, q_j and $\boldsymbol{\alpha}_k$ into their $1d$ pendants.

$$(4.15) \qquad \dot{\epsilon}_i^{in} = \lambda_k \, n_i \quad k = 1, \ldots, n_C, \quad i \in \mathrm{set}_f(k),,$$

or, in a compact way

$$(4.16) \qquad \dot{\boldsymbol{\epsilon}}^{in} = \boldsymbol{\lambda}^{(m)} \, \boldsymbol{n} = \left((\mathbb{C}^f)^T \boldsymbol{\lambda} \right) \frac{\boldsymbol{S} - \boldsymbol{x}}{|\boldsymbol{S} - \boldsymbol{x}|} \left(\frac{|\boldsymbol{S} - \boldsymbol{x}|}{(\mathbb{C}^f)^T \left(\mathbb{C}^f |\boldsymbol{S} - \boldsymbol{x}|^\beta \right)^{\frac{1}{\beta}}} \right)^{\beta - 1}.$$

The multiplication between the vector $\boldsymbol{\lambda}^{(m)}$ and the "vector with matrix components" $\boldsymbol{n}$ is component-wise. To underline this, there are brackets around $(\mathbb{C}^f)^T \boldsymbol{\lambda}$. The plastic multipliers λ_k have to fulfil the conditions (3.54) now with the yield functions in the form (4.11).

The evolution equations for q_i and $\overline{R}_i$ remain the same as in (3.65) and (3.66), respectively. In the evolution equations for α_i and $\overline{\boldsymbol{X}}_i$ (3.65) and (3.89), respectively, the factor $\frac{3}{2}$ turns out. For completeness,

we repeat these equations in their matrix-based form.

$$(4.17) \qquad \dot{\boldsymbol{q}} = \boldsymbol{\lambda}^{(q)} - \Lambda^{(q)} \, \boldsymbol{b} \, \Lambda^{(q)} \, \overline{R},$$

$$(4.18) \qquad \dot{\overline{R}} = \boldsymbol{Q} \Big(\boldsymbol{\lambda}^{(q)} - \Lambda^{(q)} \, \boldsymbol{b} \, \Lambda^{(q)} \, \overline{R} \Big) + \dot{\theta} \big(\frac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}\theta} \big) \boldsymbol{q},$$

$$(4.19) \qquad \dot{\boldsymbol{\alpha}} = (\mathbb{C}^{\alpha})^{T} \dot{\boldsymbol{\epsilon}}^{in} - \Lambda^{(\alpha)} \Big(\boldsymbol{d}^{(x)} \, \Lambda^{(\alpha)} \, \overline{\boldsymbol{x}} + \boldsymbol{d}^{(\alpha)} \, \Lambda^{(\alpha)} \, \boldsymbol{\alpha} \Big),$$

$$(4.20) \qquad \dot{\overline{\boldsymbol{x}}} = \boldsymbol{c} \left((\mathbb{C}^{\alpha})^{T} \dot{\boldsymbol{\epsilon}}^{in} - \Lambda^{(\alpha)} \Big(\boldsymbol{d}^{(x)} \, \Lambda^{(\alpha)} \, \overline{\boldsymbol{x}} + \boldsymbol{d}^{(\alpha)} \, \Lambda^{(\alpha)} \, \boldsymbol{\alpha} \Big) \right) + \dot{\theta} \big(\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}\theta} \big) \boldsymbol{\alpha},$$

$$(4.21) \qquad \dot{\boldsymbol{x}} = \mathbb{C}^{\alpha} \dot{\overline{\boldsymbol{x}}},$$

$$(4.22) \qquad \dot{\boldsymbol{R}} = \mathbb{C}^{q} \dot{\overline{\boldsymbol{R}}}.$$

Based on the equivalence hypothesis, the material parameters involved in the $3d$ equations and in their $1d$ counterparts have the same meaning, e.g. in (3.88) and (4.19).

Remark 4.1. Based on (3.52), (4.2) - (4.6), in the *current uniaxial setting*, the unit tensors $\boldsymbol{m}_i$ are

$$(4.23) \qquad \boldsymbol{m}_i = \sqrt{\frac{2}{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}, \qquad\qquad i = 1, \ldots, n_M.$$

Therefore, $\overline{\boldsymbol{X}}_i$, $\boldsymbol{\alpha}_i$ and $\boldsymbol{m}_i$ are collinear. Hence, the projections onto $\boldsymbol{m}_i$ in the evolution equations (3.86) *do not have any effect*, and it is sufficient to deal only with the approach (3.88) (that means with (4.19) in uniaxial setting.

4.2 Post-processing of measured data

As already stated, in uniaxial experiments with small probes, spatial homogeneity is usually assumed, at least over the gauge length. As a consequence, all (measured and calculated) quantities concerning these probes are only functions of time t. Thus it holds

$$(4.24) \qquad\qquad\qquad \operatorname{div} \boldsymbol{\sigma} = 0.$$

Therefore, if neglecting inertial and outer forces (like gravity), (4.24) is indeed the equation of linear momentum (2.1).

Let θ, l, d and S be measured temperature, length, diameter and applied stress, respectively, as discrete functions of time t of small cylindrical (metal) probes. Based on Hooke's law and assuming the usual homogeneity with respect to space, one obtains the subsequent equations for the (whole) longitudinal strain ϵ_L and for the (whole) transversal strain ϵ_D:

$$(4.25) \qquad \epsilon_L(t) = \frac{l(t) - l_0}{l_0} = \frac{S(t)}{E(\theta(t))} + \alpha(\theta(t) - \theta_0) + \epsilon_{in}$$

$$(4.26) \qquad \epsilon_D(t) = \frac{d(t) - d_0}{d_0} = \frac{-\nu(\theta(t)) \, S(t)}{E(\theta(t))} + \alpha(\theta(t) - \theta_0) - \frac{1}{2} \epsilon_{in}$$

l_0 and d_0 are initial length and diameter at the beginning of the essential part of the experiment (i.e., for $t = 0$). (See figure 2 for a schematic presentation.) Moreover, θ_0 is the temperature at the beginning, and, $\theta(t)$ is the temperature at time t. α is the coefficient of linear heat dilatation which is assumed to be constant in many cases. E and ν are Young's modulus and Poisson's ratio for current $\theta(t)$. As defined above, ϵ_{in} is the longitudinal inelastic, here plastic, strain. It is decomposed by (cf. 2.23))

$$(4.27) \qquad\qquad\qquad \epsilon_{in} = \sum_{i=1}^{n_M} A_i \epsilon_i^{in}.$$

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The equations (4.26) and (4.25) imply two formulas for data processing

(4.28) $\qquad \epsilon_L(t) - \epsilon_D(t) = \dfrac{(1+\nu(\theta))S(t)}{E(\theta(t))} + \dfrac{3}{2}\,\epsilon_{in},$ $\qquad$ ("strain difference"),

(4.29) $\qquad \epsilon_L(t) + 2\,\epsilon_D(t) = \dfrac{(1-2\nu(\theta))S(t)}{E(\theta(t))} + 3\alpha(\theta(t)-\theta_0)$ $\qquad$ ("volume strain").

A nice feature of the formulas (4.29) and (4.28) is that isotropic and anisotropic effects are separated. Thus, from (4.28) one gets a formula for obtaining the (whole) inelastic longitudinal strain ϵ_{in} from measured data

(4.30) $\qquad\qquad \epsilon_{in}(t) = \dfrac{2}{3}\,(\epsilon_L(t) - \epsilon_D(t)) - \dfrac{2(1+\nu(\theta))S(t)}{3E(\theta(t))}.$

Besides, formula (4.29) does not contain the inelastic strain ϵ_{in}. Thus, this formula can be used for determining the heat-dilatation coefficient α.

Unfortunately, sometimes only the longitudinal strain can be measured. In this case, the formula (4.25) is being used directly:

(4.31) $\qquad\qquad \epsilon_{in} = \epsilon_L(t) - \dfrac{S(t)}{E(\theta(t))} - \alpha\,(\theta(t)-\theta_0).$

Clearly, α must be known, or the experiments must be performed under isothermal conditions.

Remarks 4.2. (i) In general cases, if phase transformations occur, the density also depends on the phase fractions $p = (p_1, \dots, p_{N_p})$ ($N_p \geq 1$ - number of phases, cf. Wolff et al. [2012b] for details in this context). In this case, instead of the term $\alpha(\theta(t) - \theta_0)$ in (4.25) and (4.26) there must be the root

(4.32) $\qquad\qquad \sqrt[3]{\dfrac{\varrho_0}{\varrho(\theta(t), p(t))}} - 1.$

Using the relation between densities and phase fractions, the formula (4.29) can be used for determining the evolution of the phase fraction.

(ii) In case of no phase transformations, a linearization of the root in (4.32) gives

(4.33) $\qquad\qquad \sqrt[3]{\dfrac{\varrho_0}{\varrho(\theta(t))}} - 1 \approx \dfrac{\varrho_0 - \varrho(\theta(t))}{3\varrho_0} \approx -\dfrac{1}{3\varrho_0}\dfrac{\mathrm{d}\varrho}{\mathrm{d}\theta}(\theta_0)(\theta-\theta_0).$

Thus, approximately we have

(4.34) $\qquad\qquad \alpha = -\dfrac{1}{3\varrho_0}\dfrac{\mathrm{d}\varrho}{\mathrm{d}\theta}(\theta_0).$

(iii) Based on (4.2) and (2.8) and taking the relations between the elastic parameters

(4.35) $\qquad\qquad \dfrac{1}{3\,K} = \dfrac{1-2\,\nu}{E}, \qquad\qquad\qquad \dfrac{1}{2\,\mu} = \dfrac{1+\nu}{E}.$

into account, the equations (4.25) and (4.26) are in accordance with (2.18).

4.3 Semi-implicit algorithms for simulations of direct problems

Two methods are possible dealing with the discretized forward problem of spatially homogenous uniaxial material behavior: the strain-driven and the stress-driven approach.

•   Direct problem: Strain-driven approach (see Subsection 4.3.1)

The longitudinal and transversal strains are given as discrete functions of time. Sometimes, only the longitudinal strain is given. In the non-isothermal case, the temperature is given, too. Knowing the material behavior (i.e. material laws and parameters), one wishes to calculate the material response, i.e. stress, inelastic strains, back stresses etc. Thus, the strain-driven approach allows the simulation of strain-controlled experiments.

•   Direct problem: Stress-driven approach (see Subsection 4.3.2)

Now, the uniaxial stress is given as a discrete function of time. Moreover, in the non-isothermal case, the temperature is given. Calculating the material response in this context means finding the inelastic longitudinal strain corresponding to traceless phenomena like plasticity. If one wishes to simulate the *whole* longitudinal (and transversal) strain, one generally must have additional information, for instance, the heat-dilatation coefficient. Hence, the stress-driven approach allows the simulation of stress-controlled experiments, in ratcheting e.g.

    Let the $n_M n_C$ multi-mechanism model be given by its three structural matrices $\mathbb{C}^\alpha$, $\mathbb{C}^f$, $\mathbb{C}^q$ as well as by the structural vector $\boldsymbol{A} = (A_1, \ldots, A_{n_M})$ (see (3.152) – (3.154)). Moreover, there are given Young's modulus E, Poisson's ratio ν, the origin yield stresses σ_{0k} ($k = 1, \ldots, n_C$) as well as the matrices $\boldsymbol{c}$ and $\boldsymbol{Q}$ describing kinematic and isotropic hardening, respectively. All these parameters may depend on temperature. Finally, the matrices of material parameters $\boldsymbol{b}$, $\boldsymbol{d}^{(x)}$ and $\boldsymbol{d}^{(\alpha)}$ governing the evolution equations of internal variables are given, too. Besides, the parameters of these last three matrices may depend on further quantities.

4.3.1 Direct problem: Strain-driven approach

At the beginning of the nth time step, only the longitudinal and transversal strains ϵ_L^n and ϵ_D^n and possibly the temperature θ^n are given. The corresponding stress S^n and inelastic strains ϵ_{in}^n, ϵ_i^n ($i = 1, \ldots, n_M$) have to be calculated, using the concrete equations governing the material behavior.

    We develop the main steps of the algorithm, using the matrix-based approach. This means in particular, that we perform a formal update of all quantities in every time step. If some plastic multipliers are zero, clearly, the update gives the former values for the corresponding quantities. Our approach follows well-known items used in computational plasticity like return-mapping strategy (see Simo and Hughes [1998], e.g., for details).

•   **Trial, corrected and effective stresses**

Based on (4.28) we define the trial scalar stress S_{trial}^n as well as the vector $\boldsymbol{S}_{trial}^n$ of trial partial stresses.

$$(4.36) \qquad S_{trial}^n := \frac{E_n}{1 + \nu_n}(\epsilon_L^n - \epsilon_D^n - \frac{3}{2}\,\epsilon_{in}^{n-1}), \qquad\qquad \boldsymbol{S}_{trial}^n := S_{trial}^n\,\boldsymbol{A}^T,$$

with the abbreviations $E_n = E(\theta^n)$, $\nu_n = \nu(\theta^n)$.

    In a strain-driven approach, the trial stresses can be calculated directly from the measured data and former values. The true stress (of the nth time step) is a-priori unknown. It is looked for as as corrected stress S^n which is defined as follows.

$$(4.37) \quad S^n = \frac{E_n}{1+\nu_n}(\epsilon_L^n - \epsilon_D^n - \frac{3}{2}\,\epsilon_{in}^n) = \frac{E_n}{1+\nu_n}(\epsilon_L^n - \epsilon_D^n - \frac{3}{2}\,\epsilon_{in}^{n-1}) - \frac{3E_n}{2(1+\nu_n)}(\epsilon_{in}^n - \epsilon_{in}^{n-1}) =$$

$$= S_{trial}^n - \frac{3E_n\,\tau_n}{2(1+\nu_n)}\sum_{i=1}^{n_M} A_i(\dot{\epsilon}_i^{in})^n = S_{trial}^n - \tau_n\,e_n\,\boldsymbol{A}(\dot{\boldsymbol{\epsilon}}^{in})^n.$$

Clearly, the product $\boldsymbol{A}(\dot{\boldsymbol{\epsilon}}^{in})^n$ is the scalar product equivalently expressed by a matrix product of a row and a column vector. The abbreviation $e_n := \frac{3E_n}{2(1+\nu_n)}$ is used, and the difference strain $\epsilon_{in}^n - \epsilon_{in}^{n-1}$ has been approximated by

$$(4.38) \qquad\qquad\qquad\qquad \epsilon_{in}^n - \epsilon_{in}^{n-1} = \tau_n(\dot{\epsilon}_i^{in})^n,$$

with the time step $\tau_n := t_n - t_{n-1}$. A suitable approximation $(\dot{\epsilon}_i^{in})^n$ of the rate of the ith strain will be given in the next step of the algorithm. Thus, the vector of corrected partial stresses $\boldsymbol{S}^n$ reads as

$$(4.39) \qquad\qquad\qquad\qquad \boldsymbol{S}^n := S^n\,\boldsymbol{A}^T.$$

For further use, we define the vector $\boldsymbol{\xi}^n$ of effective stresses:

$$(4.40) \qquad\qquad\qquad\qquad \boldsymbol{\xi}^n := \boldsymbol{S}^n - \boldsymbol{x}^n.$$

The back stresses $\boldsymbol{x}^n = (x_1, \ldots, x_{n_M})$ are also a-priori unknown, and they must be determined during the algorithm. From (4.37) and (4.21) we get the following equation which is important for future use.

$$(4.41) \qquad\qquad \boldsymbol{\xi}^n = \boldsymbol{S}^n - \boldsymbol{x}^n = \boldsymbol{S}_{trial}^n - \tau_n\,e_n\left\{\boldsymbol{A}(\dot{\boldsymbol{\epsilon}}^{in})^n\right\}\boldsymbol{A}^T - \mathbb{C}^\alpha\overline{\boldsymbol{x}}^n.$$

Remark 4.3. If only the longitudinal strains ϵ_L^n are available, the trial stress builds up on the basis of formula (4.31):

$$(4.42) \qquad\qquad S_{trial}^n = E_n(\epsilon_L^n - \epsilon_{in}^{n-1}) - E_n\,\alpha\,(\theta^n - \theta_0).$$

clearly, the approach for the corrected stress has to modified analogously.

- **Approximation of the inelastic strain rates $(\dot{\epsilon}_i^{in})^n$**

  Based on (4.16), (4.40), we set

$$(4.43) \qquad\qquad (\dot{\boldsymbol{\epsilon}}^{in})^n = \left((\mathbb{C}^f)^T\boldsymbol{\lambda}^n\right)\frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|}\left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T\left(\mathbb{C}^f|\boldsymbol{\xi}^n|^\beta\right)^{\frac{1}{\beta}}}\right)^{\beta-1}.$$

The vector $\boldsymbol{\lambda}^n$ of plastic multipliers of the nth time step is also a-priori unknown. As we will see later on, the algorithm yields a coupled system for determining $\boldsymbol{\xi}^n$ and $\boldsymbol{\lambda}^n$. The operations in (4.43) are understood as component-wise. To underline this, there are brackets around $(\mathbb{C}^f)^T\boldsymbol{\lambda}^n$. The material parameter β may depend on temperature and other quantities. For a better overview we will drop this here.

- **Approaches for the internal variables, isotropic hardening stresses and back stresses**

These a-priori unknown quantities will be approximated by semi-implicit approaches, using (4.17) – (4.22).

$$(4.44) \qquad \boldsymbol{q}^n = \boldsymbol{q}^{n-1} + \tau_n (\mathbb{C}^q)^T \boldsymbol{\lambda}^n - \tau_n (\Lambda^{(q)})^{n-1} \boldsymbol{b}^{n-1} (\Lambda^{(q)})^{n-1} \overline{R}^{n-1},$$

$$(4.45) \qquad \overline{R}^n = \overline{R}^{n-1} + \tau_n \boldsymbol{Q}^n (\mathbb{C}^q)^T \boldsymbol{\lambda}^n - \tau_n \boldsymbol{Q}^n (\Lambda^{(q)})^{n-1} \boldsymbol{b}^{n-1} (\Lambda^{(q)})^{n-1} \overline{R}^{n-1} +$$
$$+ \left(\boldsymbol{Q}^n - \boldsymbol{Q}^{n-1} \right) \boldsymbol{q}^{n-1},$$

$$(4.46) \qquad \boldsymbol{\alpha}^n = \boldsymbol{\alpha}^{n-1} + \tau_n (\mathbb{C}^\alpha)^T (\dot{\boldsymbol{\epsilon}}^{in})^n +$$
$$- \tau_n (\Lambda^{(\alpha)})^{n-1} \Big((\boldsymbol{d}^{(x)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \overline{\boldsymbol{x}}^{n-1} + (\boldsymbol{d}^{(\alpha)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \boldsymbol{\alpha}^{n-1} \Big),$$

$$(4.47) \qquad \overline{\boldsymbol{x}}^n = \overline{\boldsymbol{x}}^{n-1} + \tau_n \boldsymbol{c}^n (\mathbb{C}^\alpha)^T (\dot{\boldsymbol{\epsilon}}^{in})^n +$$
$$- \tau_n (\Lambda^{(\alpha)})^{n-1} \Big((\boldsymbol{d}^{(x)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \overline{\boldsymbol{x}}^{n-1} + (\boldsymbol{d}^{(\alpha)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \boldsymbol{\alpha}^{n-1} \Big) +$$
$$+ \left(\boldsymbol{c}^n - \boldsymbol{c}^{n-1} \right) \boldsymbol{\alpha}^{n-1},$$

$$(4.48) \qquad \boldsymbol{R}^n = \mathbb{C}^q \overline{\boldsymbol{R}}^n, \qquad \boldsymbol{x}^n = \mathbb{C}^\alpha \overline{\boldsymbol{x}}^n.$$

Thus, semi-implicit means that only the current values of the linear terms are taken. In other words, in case of linear hardening under isothermal conditions, these approaches would be fully implicit.

- **Modified equation of effective stress**

From (4.41), (4.47) and (4.48) we obtain:

$$(4.49) \qquad \boldsymbol{\xi}^n = \boldsymbol{y}^n - \tau_n e_n \left(\boldsymbol{A} (\dot{\boldsymbol{\epsilon}}^{in})^n \right) \boldsymbol{A}^T - \tau_n \mathbb{C}^\alpha \boldsymbol{c} (\mathbb{C}^\alpha)^T (\dot{\boldsymbol{\epsilon}}^{in})^n.$$

The abbreviation $\boldsymbol{y}^n$ collects all arising term from the former time step, i.e. we set:

$$(4.50) \qquad \boldsymbol{y}^n := \boldsymbol{S}^n_{trial} - \mathbb{C}^\alpha \overline{\boldsymbol{x}}^{n-1} + \tau_n \mathbb{C}^\alpha (\Lambda^{(\alpha)})^{n-1} (\boldsymbol{d}^{(x)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \overline{\boldsymbol{x}}^{n-1} +$$
$$+ \tau_n \mathbb{C}^\alpha (\Lambda^{(\alpha)})^{n-1} (\boldsymbol{d}^{(\alpha)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \boldsymbol{\alpha}^{n-1} - \mathbb{C}^\alpha \left(\boldsymbol{c}^n - \boldsymbol{c}^{n-1} \right) \boldsymbol{\alpha}^{n-1}.$$

Now, via (4.43) the inelastic strain rates can be eliminated, obtaining an equation which contains only the unknowns $\boldsymbol{\xi}^n$ and $\boldsymbol{\lambda}^n$.

$$(4.51) \qquad \boldsymbol{\xi}^n = \boldsymbol{y}^n - \tau_n e_n \left\{ \boldsymbol{A} \left((\mathbb{C}^f)^T \boldsymbol{\lambda}^n \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T (\mathbb{C}^f |\boldsymbol{\xi}^n|^\beta)^{\frac{1}{\beta}}} \right)^{\beta-1} \right) \right\} \boldsymbol{A}^T +$$
$$- \tau_n \mathbb{C}^\alpha \boldsymbol{c} (\mathbb{C}^\alpha)^T \left((\mathbb{C}^f)^T \boldsymbol{\lambda}^n \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T (\mathbb{C}^f |\boldsymbol{\xi}^n|^\beta)^{\frac{1}{\beta}}} \right)^{\beta-1} \right).$$

The quantity inside of the parenthesis $\{\}$ is a scalar.

- **Determination of active mechanisms**

Generally, there are n_C flow criteria. Hence, we have to ask whether the following relations are fulfilled (see (3.35)).

$$(4.52) \qquad f_k(S^n_{trial,i}, x^{n-1}_i, R^{n-1}_k, R_{0k}(\theta^n)) =$$
$$= \left(\sum_{j \in \text{set}_f(k)} |S^n_{trial,j} - x^{n-1}_j|^\beta \right)^{\frac{1}{\beta}} - (R^{n-1}_k + R_{0k}(\theta^n)) \leq 0$$
$$k = 1, \ldots, n_C, \qquad i \in \text{set}_f(k).$$

The quantities $R_{0k}(\theta^n)$ are given by (see (3.41))

$$(4.53) \qquad R_{0k}(\theta^n) := \sqrt[\beta]{N_f^{(k)}}\, \sigma_{0k}(\theta^n).$$

Due to the query in (4.52), the interval $\{1, \ldots, n_C\}$ will be divided into two disjoint sets denoted by:

$$(4.54) \qquad \mathrm{set}_{no} := \{k \in \{1, \ldots, n_C\}\,|\, f_k \le 0\},$$
$$(4.55) \qquad \mathrm{set}_{yes} := \{k \in \{1, \ldots, n_C\}\,|\, f_k > 0\},$$

The subscript "no" means, that the corresponding flow criterion is not active, and the associated mechanisms do not show plastic behavior. Contrary, in case of "yes", the involved mechanisms show only thermoelastic behavior. Due to the flow conditions for the plastic multipliers () and to the evolution equations for inelastic strains and internal variables, one has

$$(4.56) \qquad \begin{array}{llll} \lambda_k = 0 & \text{for } k \in \mathrm{set}_{no}, & q_j^n = q_j^{n-1} & \text{for } j \in \mathrm{set}_q(k), \\[2mm] \epsilon_i^n = \epsilon_i^{n-1} & \text{for } i \in \mathrm{set}_f(k), & \alpha_s^n = \alpha_s^{n-1} & \text{for } s \in \mathrm{set}_\alpha(i). \end{array}$$

The λ_k for $k \in \mathrm{set}_{yes}$ must be determined, and the quantities of the associated mechanisms undergo an update.

- **Determination of plastic multipliers**

As usual in plasticity, the plastic multipliers of the active mechanisms will be determined by the corresponding flow conditions. Contrary to the query, now one uses only the current values of the n time step. Thus, using (4.9) – (4.11) and (4.40), we set

$$(4.57) \qquad \forall\, k \in \mathrm{set}_{yes} \quad : \quad f_k(\boldsymbol{S}^n, \boldsymbol{x}^n, \boldsymbol{R}^n, \boldsymbol{R}_0^n) = \left(\left(\mathbb{C}^f(|\boldsymbol{\xi}|^n)^\beta\right)^{\frac{1}{\beta}}\right)_k - (R_k^n + R_{0k}^n) = 0$$

Using (4.48) and the approximation (4.45), we get

$$(4.58) \qquad \boldsymbol{R}^n + \boldsymbol{R}_0^n = \boldsymbol{z}^n + \tau_n\, \mathbb{C}^q \boldsymbol{Q}(\mathbb{C}^q)^T \boldsymbol{\lambda}^n,$$

where the vector $\boldsymbol{z}^n$ collects all term not containing current values:

$$(4.59) \qquad \boldsymbol{z}^n := \boldsymbol{R}_0^n - \tau_n \mathbb{C}^q \boldsymbol{Q}^n (\Lambda^{(q)})^{n-1}\, \boldsymbol{b}^{n-1}\, (\Lambda^{(q)})^{n-1}\, \overline{R}^{n-1} + \mathbb{C}^q \big(\boldsymbol{Q}^n - \boldsymbol{Q}^{n-1}\big) \boldsymbol{q}^{n-1}.$$

Since the multipliers belonging to the non-active mechanisms are zero, we have to solve a reduced system of equations for the multipliers of the active mechanisms. For this reason we define an auxiliary diagonal matrix $\boldsymbol{H}_{yes}^n$ by

$$(4.60) \qquad \boldsymbol{H}_{yes}^n \in \{0,1\}^{n_C \times n_C}, \qquad (\boldsymbol{H}_{yes}^n)_{ij} := \begin{cases} 1, & \text{if } i = j \ \text{ and } f_j > 0, \\ 0, & \text{otherwise.} \end{cases}$$

Now, the reduced system of equations for determining the modified vector $\boldsymbol{\lambda}_{mod}^n$ defined by

$$(4.61) \qquad \boldsymbol{\lambda}_{mod}^n := \boldsymbol{H}_{yes}^n\, \boldsymbol{\lambda}^n$$

can be written down using the items provided before.

$$(4.62) \qquad \boldsymbol{H}_{yes}^n \left(\mathbb{C}^f(|\boldsymbol{\xi}|^n)^\beta\right)^{\frac{1}{\beta}} = \boldsymbol{H}_{yes}^n\, \boldsymbol{z}^n + \tau_n\, \boldsymbol{H}_{yes}^n \mathbb{C}^q \boldsymbol{Q}(\mathbb{C}^q)^T \boldsymbol{\lambda}_{mod}^n.$$

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In Subsection 3.2, the matrix $\boldsymbol{Q}$ of isotropic hardening moduli has been assumed to be positive semidefinite (see (3.30)). Under the additional assumption

(4.63) $$\det(\boldsymbol{Q}) > 0$$

the equation (4.62) can be solved with respect to $\boldsymbol{\lambda}_{mod}^n$. As a result, one gets

(4.64) $$\boldsymbol{\lambda}_{mod}^n = \frac{1}{\tau_n} \boldsymbol{L}^n \, \boldsymbol{H}_{yes}^n \big\{ \big(\mathbb{C}^f (|\boldsymbol{\xi}|^n)^\beta \big)^{\frac{1}{\beta}} - \boldsymbol{z}^n \big\},$$

where the abbreviation

(4.65) $$\boldsymbol{L}^n := \big(\boldsymbol{H}_{yes}^n \mathbb{C}^q \boldsymbol{Q} (\mathbb{C}^q)^T \big)^{-1}$$

has been used.

- **Calculation of effective stresses and plastic multipliers**

Inserting the expressing for $\boldsymbol{\lambda}_{mod}^n$ into the equation (4.51), we obtain the following non-linear system for determining the effective stresses $\boldsymbol{\xi}^n$.

(4.66) $\boldsymbol{\xi}^n = \boldsymbol{y}^n +$

$$- e_n \left\{ \boldsymbol{A} \left((\mathbb{C}^f)^T \boldsymbol{L}^n \, \boldsymbol{H}_{yes}^n \big\{ \big(\mathbb{C}^f (|\boldsymbol{\xi}|^n)^\beta \big)^{\frac{1}{\beta}} - \boldsymbol{z}^n \big\} \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T \big(\mathbb{C}^f |\boldsymbol{\xi}^n|^\beta \big)^{\frac{1}{\beta}}} \right)^{\beta-1} \right) \right\} \boldsymbol{A}^T +$$

$$- \mathbb{C}^\alpha \boldsymbol{c} (\mathbb{C}^\alpha)^T \left((\mathbb{C}^f)^T \boldsymbol{L}^n \, \boldsymbol{H}_{yes}^n \big\{ \big(\mathbb{C}^f (|\boldsymbol{\xi}|^n)^\beta \big)^{\frac{1}{\beta}} - \boldsymbol{z}^n \big\} \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T \big(\mathbb{C}^f |\boldsymbol{\xi}^n|^\beta \big)^{\frac{1}{\beta}}} \right)^{\beta-1} \right).$$

This non-linear system has to be solved by an iteration procedure (by Newton's approach, e.g.). In the special case of $n_M n_C$ models with $n_M = n_C$ (i.e., each mechanism has its own flow criterion), the system will be considerably simplified. This yields

(4.67) $$\boldsymbol{\xi}^n = \boldsymbol{y}^n - e_n \left\{ \boldsymbol{A} \left(\boldsymbol{L}^n \, \boldsymbol{H}_{yes}^n \big\{ |\boldsymbol{\xi}|^n - \boldsymbol{z}^n \big\} \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \right) \right\} \boldsymbol{A}^T +$$

$$- \mathbb{C}^\alpha \boldsymbol{c} (\mathbb{C}^\alpha)^T \left(\boldsymbol{L}^n \, \boldsymbol{H}_{yes}^n \big\{ |\boldsymbol{\xi}|^n - \boldsymbol{z}^n \big\} \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \right).$$

Finally, knowing $\boldsymbol{\xi}^n$, the plastic multipliers $\boldsymbol{\lambda}^n = \boldsymbol{\lambda}_{mod}^n$ can be obtained by (4.64).

- **Updates of stress, inelastic strain, internal variables and back stresses**

After calculating the effective stresses and plastic multipliers, the remaining quantities will be updated in the following way. Using (4.43), we obtain the rates of inelastic partial strains $(\dot{\boldsymbol{\epsilon}}^{in})^n$ as well as the full inelastic longitudinal strain $(\epsilon_{in})^n$ by

(4.68) $$(\epsilon_{in})^n = (\epsilon_{in})^{n-1} + \tau_n \, \boldsymbol{A} (\dot{\boldsymbol{\epsilon}}^{in})^n.$$

Moreover, the stress S^n follows from (4.37). Finally, the quantities $\boldsymbol{q}^n$, $\overline{\boldsymbol{R}}^n$, $\boldsymbol{R}^n$, $\boldsymbol{\alpha}^n$, $\overline{\boldsymbol{x}}^n$ and $\boldsymbol{x}^n$ will be updated with the help of (4.44) – (4.48).

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4.3.2 Direct problem: Stress-driven approach

Contrary to the strain-driven approach in Subsection 4.3.1, now, at the beginning of the nth time step, only the stress S^n and possibly the temperature θ^n are given. The longitudinal and transversal strains ϵ_L^n and ϵ_D^n as well as the inelastic strains ϵ_{in}^n, ϵ_i^n $(i = 1, \ldots, n_M)$ have to be calculated. Some of the approaches presented before in the strain-driven approach remain the same. For this reason, we will deal in short with the algorithm.

Since now the stress S^n is given, we start with (4.39) and (4.40) and obtain (cf. (4.41))

$$(4.69) \qquad \boldsymbol{\xi}^n = \boldsymbol{S}^n - \boldsymbol{x}^n = \boldsymbol{S}^n - \mathbb{C}^\alpha \overline{\boldsymbol{x}}^n.$$

The back stresses $\overline{\boldsymbol{x}}^n = (x_1, \ldots, x_{nualpha})$ are a-priori unknown. Thus, the effective stresses $\boldsymbol{\xi}^n$ are also a-priori unknown. The inelastic strain rates $(\dot{\boldsymbol{\epsilon}}^{in})^n$ as well as $\boldsymbol{q}^n$, $\overline{\boldsymbol{R}}^n$, $\boldsymbol{R}^n$, $\boldsymbol{\alpha}^n$, $\overline{\boldsymbol{x}}^n$ and $\boldsymbol{x}^n$ will be discretized as in (4.43) and (4.44) – (4.48). Thus, from (4.69) we obtain an analogous but simpler equation for the unknowns $\boldsymbol{\xi}^n$ and $\boldsymbol{\lambda}^n$.

$$(4.70) \qquad \boldsymbol{\xi}^n = \boldsymbol{y}^n - \tau_n \mathbb{C}^\alpha \boldsymbol{c}(\mathbb{C}^\alpha)^T \left((\mathbb{C}^f)^T \boldsymbol{\lambda}^n \frac{\boldsymbol{\xi}^n}{|\boldsymbol{\xi}^n|} \left(\frac{|\boldsymbol{\xi}^n|}{(\mathbb{C}^f)^T \left(\mathbb{C}^f |\boldsymbol{\xi}^n|^\beta \right)^{\frac{1}{\beta}}} \right)^{\beta-1} \right),$$

where $\boldsymbol{y}^n$ is given by

$$(4.71) \qquad \boldsymbol{y}^n := \boldsymbol{S}^n - \mathbb{C}^\alpha \overline{\boldsymbol{x}}^{n-1} + \tau_n \mathbb{C}^\alpha (\Lambda^{(\alpha)})^{n-1} (\boldsymbol{d}^{(x)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \overline{\boldsymbol{x}}^{n-1} +$$

$$+ \tau_n \mathbb{C}^\alpha (\Lambda^{(\alpha)})^{n-1} (\boldsymbol{d}^{(\alpha)})^{n-1} (\Lambda^{(\alpha)})^{n-1} \boldsymbol{\alpha}^{n-1} - \mathbb{C}^\alpha (\boldsymbol{c}^n - \boldsymbol{c}^{n-1}) \boldsymbol{\alpha}^{n-1}.$$

The determination of the active mechanisms is as before. The only difference is that now the given stress will be used in the query (instead of the trial one in the strain-driven approach, cf. (4.52)). Thus, we have the same equations (4.64) for the plastic multipliers. Inserting these equations into (4.70), the effective stresses $\boldsymbol{\xi}^n$ can be calculated as above by an iteration scheme. The updates of $(\epsilon_{in})^n$, $\boldsymbol{q}^n$, $\overline{\boldsymbol{R}}^n$, $\boldsymbol{R}^n$, $\boldsymbol{\alpha}^n$, $\overline{\boldsymbol{x}}^n$ and $\boldsymbol{x}^n$ can be performed as before.

Finally, the (full) longitudinal strain ϵ_L^n and the transversal strain ϵ_D^n will be obtained by

$$(4.72) \qquad \epsilon_L^n = \frac{S^n}{E_n} + \boldsymbol{A} \left(\boldsymbol{\epsilon}^{in} \right)^n,$$

$$(4.73) \qquad \epsilon_D^n = -\frac{\nu_n S^n}{E_n} - \frac{1}{2} \boldsymbol{A} \left(\boldsymbol{\epsilon}^{in} \right)^n.$$

4.4 Inverse problem: Parameter identification

The material response is known, mostly from experiments. Assuming special kinds of material laws (two mechanism with a common yield criterion, e.g.) and constant parameters in simple cases, one wants to determine these parameters in such a way that the simulated material behavior gives the best approximation of the experiment (in some sense, least square, e.g.). As pointed out in Mahnken and Stein [1996], in case of complex material behavior one needs an optimization procedure which allows a *simultaneous* determination of parameters. We will follow this approach.

In our situation, as shown in Subsection 4.2, we assume that the data θ, l, d and S are given as (discrete) functions of time stemming from experiments. In accordance with (4.25), (4.25) and (4.30), the quantities ϵ_L, ϵ_D and ϵ_{in} can be also regarded as given functions following from experimental data by simple calculations. Let the points in time be denoted by $t_0 < t_1 < \cdots < t_n < \cdots < t_N$. The corresponding values of S, θ, ϵ_L, etc. are denoted by S^n, θ^n, ϵ_L^n, etc.

When performing parameter identification via a strain-driven approach, in the nth time step, the values ϵ_L^n, ϵ_D^n (and sometimes θ^n) are regarded as given. The stress S^n, the inelastic strain ϵ_{in}^n and possibly other quantities must be calculated. The optimization procedure compares this calculated stress S^n with the experimentally measured one S_{ex}^n. Additionally, the calculated inelastic strain can be compared with the experimentally obtained one.

Contrary, during parameter identification via a stress-driven approach, the values S^n (and possibly θ^n) are assumed as given, and the inelastic strain ϵ_{in}^n must be calculated. The optimization procedure compares the calculated value ϵ_{in}^n with the experimentally found one $\epsilon_{in,ex}^n$.

Finally, it is possible to combine the strain-driven and stress-driven approach in one optimization routine. We introduce some notations: Let the following data base

$$(4.74) \qquad \left(\epsilon_L^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(\epsilon_D^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(S^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(\theta^{n,j}\right)_{n=1,j=1}^{N_j,J}$$

be given from uniaxial experiments. J is the number of experiments, $N_j > 1$ is the number of instants of time of the jth experiment. The matrix $\left(\epsilon_{in}^{n,j}\right)_{n=1,j=1}^{N_j,J}$ can easily be calculated by (4.30 or by (4.31). Hence, it can be considered as given, too. After this, a suitable set of (generally vector-valued) parameters Ξ and a start value $\bar{\xi} \in \Xi$ have to be chosen.

We define functions assigning the calculated quantities to the given ones and to the parameters ξ:

$$(4.75) \qquad \left(S_{cal-strain}^{n,j}\right)_{n=1}^{N_j} := F_{strain-driven}^S\left(\left(\epsilon_L^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_D^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi\right),$$

$$(4.76) \qquad \left(\epsilon_{in,cal-strain}^{n,j}\right)_{n=1}^{N_j} := F_{strain-driven}^{\epsilon_{in}}\left(\left(\epsilon_L^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_D^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi\right),$$

$$(4.77) \qquad \left(\epsilon_{in,cal-stress}^{n,j}\right)_{n=1}^{N_j} := F_{stress-driven}^{\epsilon_{in}}\left(\left(S^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi\right),$$

with $1 \le j \le J$. The subscripts "cal-strain" and "strain-driven" mean that $\left(S_{cal}^n\right)_{n=1}^{N_j}$ and $\left(\epsilon_{in,cal}^n\right)_{n=1}^{N_j}$ are calculated by the strain-driven approach described in subsection 4.3.1, while "cal-stress" and "stress-driven" refer to the stress-driven approach presented in subsection 4.3.2.

Before the identification procedure, for each $j \in \{1, \ldots, J\}$ we define:

$$(4.78) \qquad \Phi\left(\left(\epsilon_L^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_D^{n,j}\right)_{n=1}^{N_j}, \left(S^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi, \bar{\xi}, N_j\right) =$$

$$= \overline{\Phi}\left(\left(S_{cal-strain}^{n,j}\right)_{n=1}^{N_j} - \left(S^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_{c,cal-strain}^{n,j}\right)_{n=1}^{N_j} - \left(\epsilon_c^{n,j}\right)_{n=1}^{N_j},\right.$$

$$\left.\left(\epsilon_{c,cal-stress}^{n,j}\right)_{n=1}^{N_j} - \left(\epsilon_c^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_L^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_D^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi, \bar{\xi}, N_j\right).$$

The cost functional $\overline{\Phi}$ must be chosen in a suitable way. The differences in (4.78) support the idea that the calculated values are compared with the corresponding experimental ones. Usually, the functional $\overline{\Phi}$ contains the l^p-norms, $p = 2$, of these differences ("least-square approach"). However, other exponents p between 1 and ∞ instead of 2 are possible. Moreover, $\overline{\Phi}$ is allowed to depend directly on experimental data as well as the number of time-instants. This is for reasons of suitable weighting.

In many cases, the optimization uses all data simultaneously. Thus, the "final" cost functional Ψ is the sum over all data sets:

$$(4.79) \qquad \Psi\left(\left(\epsilon_L^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(\epsilon_D^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(S^{n,j}\right)_{n=1,j=1}^{N_j,J}, \left(\theta^{n,j}\right)_{n=1,j=1}^{N_j,J}, \xi, \bar{\xi}, \left(N_j\right)_{j=1}^J\right) =$$

$$= \sum_{j=1}^J \Phi\left(\left(\epsilon_L^{n,j}\right)_{n=1}^{N_j}, \left(\epsilon_D^{n,j}\right)_{n=1}^{N_j}, \left(S^{n,j}\right)_{n=1}^{N_j}, \left(\theta^{n,j}\right)_{n=1}^{N_j}, \xi, \bar{\xi}, N_j\right).$$

We summarize the procedure in box 4.1

Remarks 4.4. (i) As explained in Subsection 3.9, the number of material parameters to be determined may be large even in case of two-mechanism models with more complexity. Note that the structural matrices $\mathbb{C}^\alpha$, $\mathbb{C}^f$ and $\mathbb{C}^q$ (see (3.154)) are given. In most cases, the "thermoelastic" parameters and quantities in (3.150) are assumed to be given. In case of necessity, they have to be determined earlier based on separate experiments. In many applications, the weighting parameters A_j (see (3.151) and (3.152)) are set equal to one. Frequently, the initial yield stresses σ_{0k} (see (3.42)) are assumed to be given. However, they can be determined simultaneously together with the remaining material parameters.

(ii) In case of an assumed temperature dependence of a material parameter m, for instance, one can set

(4.80) $$m(\theta) = m_0 + m_1\,\theta.$$

Therefore, instead of m the two constants m_0 and m_1 have to be found. Sometimes, the previously obtained value m can be used as a start value for m_0. Clearly, in this case case, one necessitates data from experiments performed at different temperatures or with varying temperature.

(iii) The routine in box 4.1 contains the strain- and stress-driven approach. More precisely, $\overline{\Phi}$ contains generally three differences. Obviously, it is possible to use only one or two of them. In case of stress-driven algorithm, we only take the difference $\left(\epsilon_{c,cal-stress}^{n,j}\right)_{n=1}^{N} - \left(\epsilon_c^{n,j}\right)_{n=1}^{N}$ into account. Principally, one can compare the difference $\left(\epsilon_L^{n,j}\right)_{n=1}^{N} - \left(\epsilon_D^{n,j}\right)_{n=1}^{N}$ of measured longitudinal and transversal strains with the differences of the calculated ones. However, due to (4.72), (4.73), this calculated strain difference and the calculated inelastic strain have the "same quality" for given stress.

5 Application to experiments in cyclic plasticity for the steel X2CrNiMo17-12-2 (1.4404)

In this Section apply theory and algorithms developed in the previous sections to data stemming from uniaxial experiments in cyclic plasticity. Our aim is to show the algorithms are applicable to experimental data. An extensive comparison of different MM models with various evolution laws is not intended.

5.1 Materials and experiments

The experimental data have been generated using specimens of the steel X2CrNiMo17-12-2 (1.4404) (see Figure 3). The chemical composition has been analyzed via SOES and is shown in Table 1.

Elements	C	Si	Mn	P	S	Cr	Mo	Ni
Mass%	0.017	0.442	1.405	0.034	0.024	16.57	2.04	10.09
	± 0.001	± 0.005	± 0.007	± 0.001	± 0.002	± 0.15	± 0.01	± 0.02
Elements	N	Cu	Co	W	V			
Mass%	0.071	0.422	0.126	0.085	0.0504			
	± 0.002	± 0.003	± 0.001	± 0.001	± 0.0004			

Table 1: Chemical composition of the steel used in the experiments
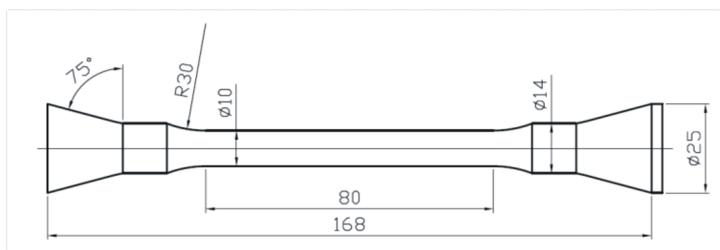
Figure 3: Cross section of a specimen for uniaxial experiments.

The mechanical behavior was investigated with tensile test specimens as shown in Fig. 3. The specimens were taken in axial direction from the semi-finished rods with a diameter of $30mm$. In order to determine the longitudinal and transversal Young's modulus five specimens were equipped with a two dimensional tactile strain sensor. Additionally, strain gauges were bond in both directions to validate the measurement of the strain sensor. The tensile tests have been performed on servo-hydraulic test equipment PSA. While loading the specimen with a strain rate of $1.4 \times 10^{-4} s^{-1}$, the current strains and loads are collected by a computer system. Table 5.1 shows the results of the tensile tests compared to the literature. Cyclic tests with 100 cycles (except one test with 70 cycles) under different loading conditions have been performed (see Tables 3 and 4).

5.2 Evaluation of some models

In order to demonstrate the applicability of the algorithms developed above we will evaluate four $n_M n_C$ models with $n_M = n_C$, using the data base listed up in Tables 3 and 4. To be more concrete, we consider the following models.

	Young's modulus (GPa)	$R_{\rho0.2}$ (MPa)	R_m (MPa)	Hardness ($HV10$)
Experiment	194 ± 4	280 ± 3	615 ± 2	165 ± 1
Literature	$200^{1)}$ and $200^{2)}$	$\geq 207^{1)}$	$517 - 655^{1)}$	$160 - 190$

Table 2: Mechanical properties of the steel X2CrNiMo17-12-2 (1.4404). [1] http://www.matweb.com, [2] Grote and Feldhusen [2007]

No.	σ_a	σ_m	N		No.	σ_a	σ_m	N		No.	σ_a	σ_m	R	N
1	250	0	100		1	115	115	100		1	210	40	-0.62	100
2	260	0	100		2	125	125	100		2	230	20	-0.84	100
3	270	0	100		3	135	135	100		3	250	0	-1	100
4	280	0	100		4	145	145	100		4	290	40	-0.72	100
5	290	0	100		5	150	150	100		5	310	20	-0.87	100
6	300	0	100		6	155	155	100		6	330	0	-1	100
7	310	0	100		7	165	165	100						
8	320	0	100		8	175	175	100						
9	330	0	100											
10	330	0	70											

Table 3: Cyclic tests with stress ratio $R = -1$ (left), with stress ratio $R = 1$ (middle) and with different stress ratios R (right). σ_a - stress amplitude (MPa), σ_m - mean stress (MPa), N - number of cycles.

No.	σ_a	σ_m	N	No.	σ_a	σ_m	N
1	210	40	40	3	210	40	40
	100	0	20		100	0	20
	210	40	40		210	-40	40
2	290	40	40	4	210	-40	40
	100	0	20		100	0	20
	290	40	40		210	40	40

Table 4: Four cyclic tests with block loading and with different stress ratios. σ_a - stress amplitude (MPa), σ_m - mean stress (MPa), N - number of cycles.

Model I: $1M$ model with two kinematic variables ("Chaboche" model) with its structural matrices (cf. (3.154))

$$\mathbb{C}^\alpha = \begin{pmatrix} 1 & 1 \end{pmatrix}, \quad \mathbb{C}^f = \begin{pmatrix} 1 \end{pmatrix}, \quad \mathbb{C}^q = \begin{pmatrix} 1 \end{pmatrix}.$$

Model II: $2M2C$ model with one kinematic variable per each mechanism and with one isotropic variable per each flow criterion

$$\mathbb{C}^\alpha = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbb{C}^f = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbb{C}^q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Model III: $2M2C$ model with two kinematic variables per one mechanism and with one per the remaining mechanism as well as with one isotropic variable per flow criterion

$$\mathbb{C}^\alpha = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{C}^f = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbb{C}^q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Model IV: $3M3C$ model with one kinematic variable per each mechanism and with one isotropic variable per each flow criterion

$$\mathbb{C}^{\alpha} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{C}^{f} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbb{C}^{q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We use the evolution equations given in (3.156) and (3.157) with constant parameter matrices $\boldsymbol{d}^{(x)}$, $\boldsymbol{d}^{(\alpha)}$ and $\boldsymbol{b}$. The matrices $\boldsymbol{Q}$, $\boldsymbol{d}^{(\alpha)}$ and $\boldsymbol{b}$ are assumed as to be diagonal. The unknown parameters are listed up in Table 5.2. For simplicity, we set $A_i = 1$ for all $i = 1, \ldots, n_M$ (see (3.151), (3.152)). The simulations have been performed with the Young's modulus of $194 GPa$ (cf. Table 5.1) and with the Poisson's ratio of 0.29. Instead of the initial yield stress $R_{\rho 0.2} = 280 MPa$ as stated in Table 5.1, we use a smaller value $R_0 = 165 MPa$ which indicates the first deviation from the line characterizing the elastic domain. This value has been determined before.

Model	$\boldsymbol{c}$	$\boldsymbol{Q}$	$\boldsymbol{d}^{(x)}$	$\boldsymbol{d}^{(\alpha)}$	$\boldsymbol{b}$	Σ
I	3	1	3	2	1	10
II	3	2	3	2	2	12
III	6	2	6	3	2	19
IV	6	3	6	3	3	21

Table 5: Number of unknown parameters of the models I - IV which must be determined, Σ is their sum. The matrices $\boldsymbol{Q}$, $\boldsymbol{d}^{(\alpha)}$ and $\boldsymbol{b}$ are assumed to be diagonal.

At first, we will find optimal parameters for each of the selected models using the group of data sets given in the middle of Table 3. After that, we will find optimal parameters for each of the selected models simultaneously taking the whole data base in Tables 3 and 4 into account. We present results for the experiment no. 4 in the middle of Table 3 ($\sigma_a = \sigma_m = 145 MPa$) (see Figure mm). Figures 5 and 6 show an experimental stress-strain curve and simulated ones based on the selected group of the data sets. Contrary to this, in the second case shown in the Figures 7 and 8 all data sets in Tables 3 and 4 have been taken into account. The results were obtained using the strain-driven approach. The simulations were performed with the programme package MATLAB. More details concerning the optimization procedure can be found in the report by Büsing and Schlasche [2013].

As already stated above, it is not the aim here to provide an exhausting comparison between different MM models using different groups of data sets. The intention is to show that the algorithms developed above are applicable and yield reasonable results. However, some careful assertions can be made. All models did not give a good approximation of the first two cycles, in particular when optimizing over the whole data base. Moreover, model I (one mechanism with two kinematic variables) does not approximate the experiment when optimizing over all data. Considering cycles with higher numbers, models II – IV yield a good approximation in both cases of the optimization approach.

6 Summary and outlook

This study deals with multi-mechanism models (MM models) in series with plastic mechanisms. The main ideas can be also applied to other material behavior. The main part, published in Section 3, provides extensions of MM models with several kinematic internal variables per mechanism as well as with several isotropic internal variables per flow criterion. The structural characterizations of these complex MM models which express the mutual relations between mechanisms, flow criteria, kinematic and isotropic
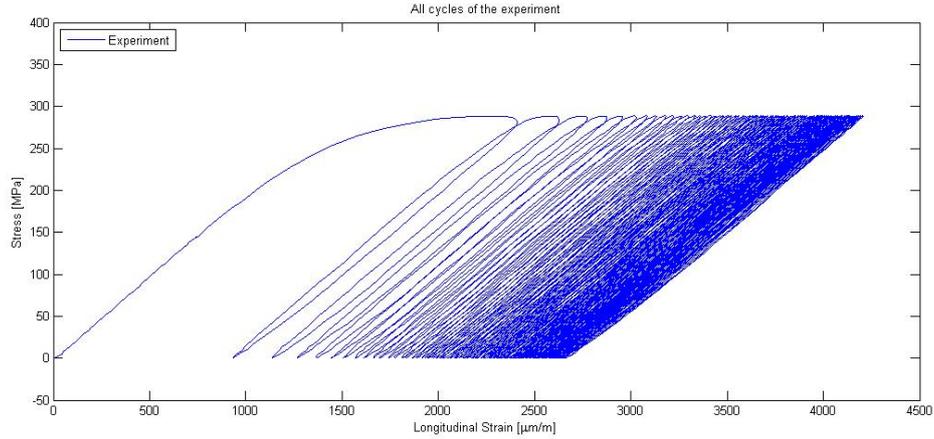
Figure 4: Stress-strain curve for all cycles of the experiment no. 4 in the middle of Table 3 ($\sigma_a = \sigma_m = 145 MPa$)
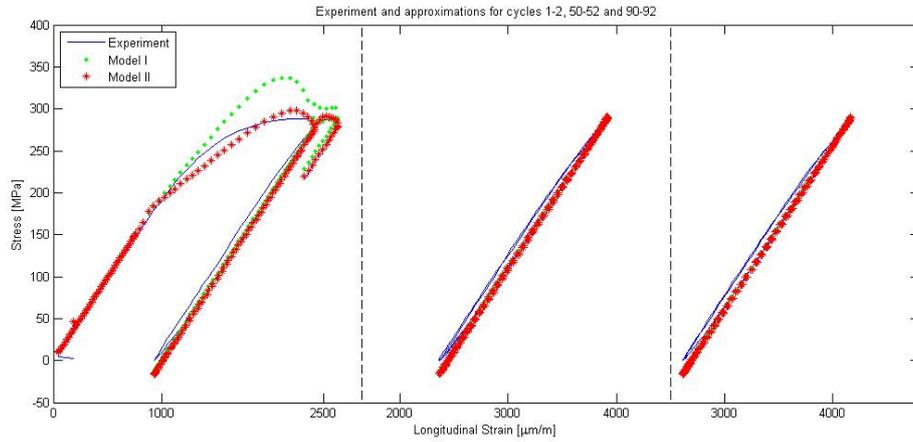
Figure 5: Stress-strain curves for the experiment no. 4 in the middle of Table 3 ($\sigma_a = \sigma_m = 145 MPa$) and comparison with simulated curves for models I and II. The optimization procedure took the group of data sets in the middle of Table 3 into account.

variables are encoded by three structure matrices (see (3.154)). Moreover, we present general evolution equations for the internal variables which allow further coupling between the mechanisms. Besides, these proposals lead to thermodynamically consistent models under reasonable sufficient conditions on the parameter functions. This general approach covers many (plasticity) models in use like one-mechanism models ("Chaboche" models, see Chaboche [2008]) and two-mechanism models (see Saï [2011], e.g.).

In the second part (Section 4), we have developed algorithms for simulation and parameter identification based on uniaxial experiments with specimens where spatial homogeneity is assumed (over the gauge length). These algorithms are matrix-based, using the three structural matrices (see (3.154)) as main input. Thus, in principal, arbitrary MM models can be dealt with in a common framework. Our approach follows well-known items used in computational plasticity like return-mapping strategy (see

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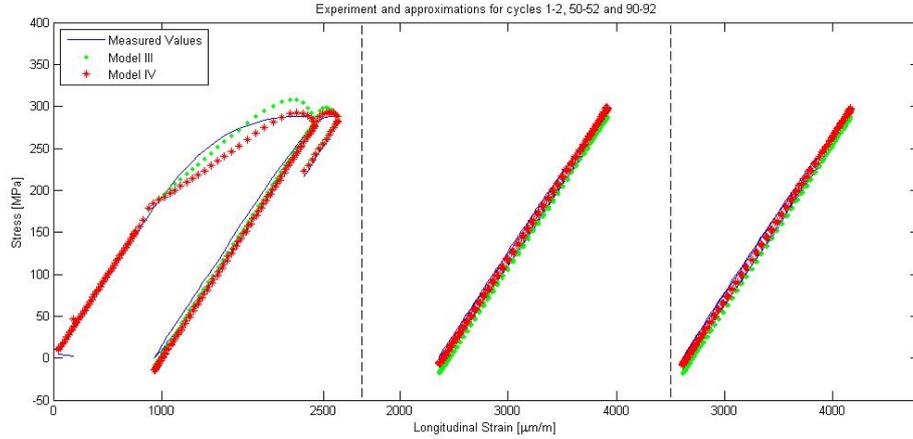
Figure 6: Stress-strain curves for the experiment no. 4 in Table 3 ($\sigma_a = \sigma_m = 145 MPa$) and comparison with simulated curves for models III and IV. The optimization procedure took the group of data sets in the middle of Table 3 into account.
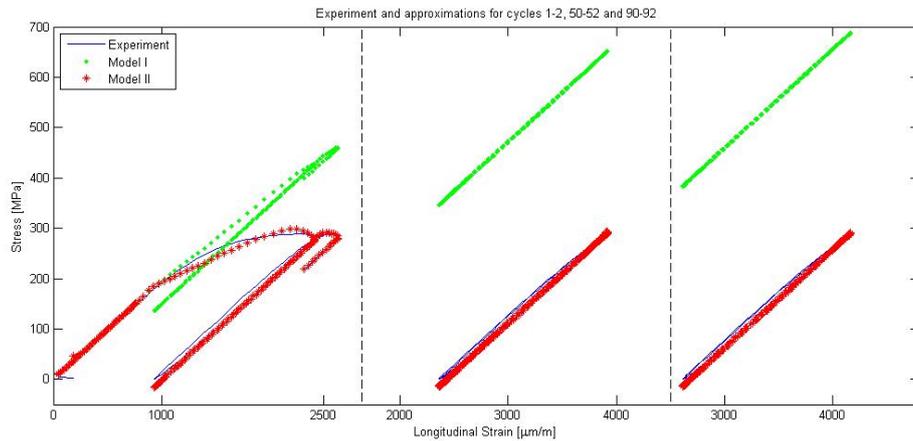
Figure 7: Stress-strain curves for the experiment no. 4 in the middle of Table 3 ($\sigma_a = \sigma_m = 145 MPa$) and comparison with simulated curves for models I and II. The optimization procedure took all data sets in the Tables 3 and 4 into account.

Simo and Hughes [1998], e.g., for details).

Finally, in the last part (Section 5), we have applied the developed algorithms to real data stemming from cyclic experiments with the steel X2CrNiMo17-12-2 (1.4404). The aim was to show the applicability of the algorithms. A detailed evaluation using different groups of data, different cost functionals as well as different optimization strategies (strain-driven, stress-driven and combined) remains for future work. Moreover, it is an open question how to fill the arising parameter matrices (fully, diagonally or with some blocks) in order to get a sufficiently good approximation and to limit the sum of parameters.

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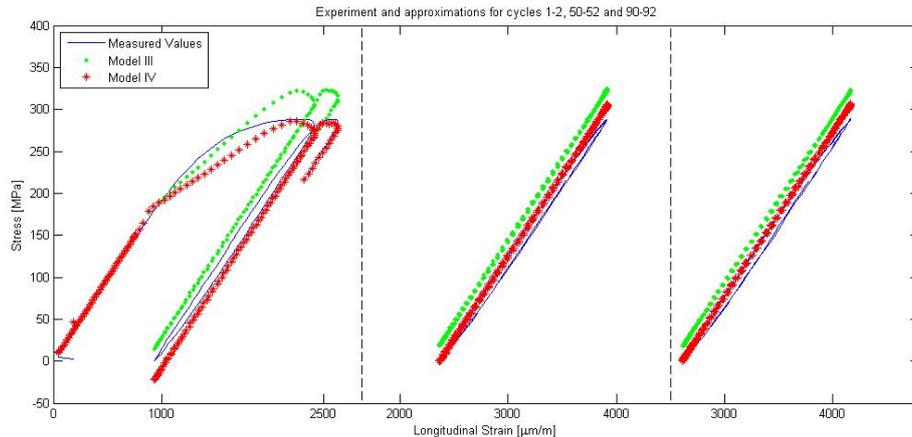
Figure 8: Stress-strain curves for the experiment no. 4 in Table 3 ($\sigma_a = \sigma_m = 145 MPa$) and comparison with simulated curves for models III and IV. The optimization procedure took all data sets in the Tables 3 and 4 into account.

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