PERGAMON

International Journal of Solids and Structures 38 (2001) 9423–9436

INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES

www.elsevier.com/locate/ijsolstr

Development of a generalized material interface for the simulation of finite elasto-plastic deformations ☆

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Received 12 May 2001

Abstract

Suitable material models have to be chosen to achieve realistic numerical simulations of the mechanical behavior of components and structures as well as a reliable identification of material parameters for finite deformations analyzing inhomogeneous displacement fields. The fundamental relations of the kinematics of an elasto-plastic continuum are formulated using the multiplicative split of the deformation gradient, the concept of dual variables and the covariance principle. A thermodynamically consistent system of differential and algebraic equations (DAE) is derived in the reference configuration to describe the rate-independent inelastic material behavior. It contains the associated flow rule, evolutional equations for the internal variables describing different kinds of hardening and the yield condition. An algorithm for the solution of the DAE based on a suitable time discretization of the differential equations is presented as well as a numerical example using the experimental FE-code PMHP on parallel computers developed at the Chemnitz University of Technology. An important advantage of the presented algorithm is its high efficiency in case of the determination of the consistent material matrix as well as within the scope of the semianalytical sensitivity analysis as a deciding part of the parameter optimization process. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Elasto-plasticity; Finite deformations; Deformation law; Thermodynamic consistency; Parameter identification

1. Introduction

The successful numerical simulation of the mechanical behavior of components and structures requires the implementation of suitable material models into finite element codes and a sufficient knowledge of the material parameters. Because the material parameters are not measurable directly, they have to be identified solving an inverse problem, which is in general approximated using nonlinear optimization methods. Within this framework an objective function containing differences of measured and calculated values of suitable variables has to be minimized. Modern identification methods analyzing inhomogeneous displacement fields have been developed by several authors for small elasto-plastic deformations (Mahnken and Stein, 1994; Gelin and Ghouati, 1995; Meuwissen, 1998) as well as for finite deformations (Mahnken

☆ Expanded version of a talk presented at the EUROMECH Colloquium 394 (Graz, March 1999).

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PII: S0020-7683(01)00131-7

and Stein, 1997; Mahnken and Kuhl, 1999). Identification procedures based on experimental results of inhomogeneous displacement fields require suitable numerical methods, like FEM, to calculate comparative values for the chosen variables.

A method to identify material parameters for small elasto-plastic deformations analyzing bending experiments with notched specimens has been developed at the Chemnitz University of Technology in the last years (Bohnsack, 1997; Görke and Kreißig, 1997). This method is a gradient based optimization procedure using a semianalytical sensitivity analysis.

The assumption of small deformations is not appropriate in a huge number of practical applications (e.g. in forming processes). This fact motivates the extension of the identification method for its application to finite deformations. Some results of our investigations in the field of the development of suitable material models and algorithms for their numerical solution including the determination of the consistent material matrix as well as the semianalytical sensitivity analysis for the parameter optimization are presented in this paper. Basic relations of a thermodynamically consistent deformation law for finite elasto-plastic deformations as a differential and algebraic equation (DAE)-system have been derived.

2. Kinematics of finite deformations

Different, and frequently controversially discussed approaches for the modeling of finite elasto-plastic deformations can be found in the literature. The main problem is the definition of elastic and plastic parts of the deformation, which in general neither can be measured separately nor can be described using physically useful kinematic quantities. Finally, several authors refer to several convenient constitutive assumptions, often phenomenological – based on geometric models of a continuum, the physics of the material (in some modern approaches microstructural) or a mixture of them. A material model should be regarded as suitable if it reflects the perceived reality with satisfying accuracy. This can be proved only by experiments.

Our approach for the establishment of elasto-plastic material models considering finite deformations is based on the multiplicative split of the deformation gradient $\boldsymbol{F} = \boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{p}}$ into an elastic part $\boldsymbol{F}^{\mathrm{e}}$ and a plastic part $\boldsymbol{F}^{\mathrm{p}}$. Following several authors (Sidoroff, 1973; Kleiber, 1975; Haupt, 1985; Simo and Ortiz, 1985; Miehe, 1992; Le and Stumpf, 1993) we assume three different configurations – the reference configuration, which usually is regarded as the undeformed one, the current configuration, which represents the mapping of the deformed body at the current time to the Euclidean space, and the so-called plastic intermediate configuration. The introduction of an intermediate configuration is controversially discussed (Lee, 1969; Green and Naghdi, 1971; Naghdi, 1990). It is well known that the plastic intermediate configuration is not a compatible physical one in the sense of an elastically unloaded configuration, and that the elastic and plastic parts of the deformation gradient are not really gradients of certain mappings of manifolds in contrast to the deformation gradient itself. We consider the plastic intermediate configuration as a convenient tool to formulate some useful kinematical quantities similar to those which are defined in the reference and current configurations.

Some covariant strain tensors as well as their elastic and plastic parts can be defined using the deformation gradient and its constitutive parts. Here and in the following we denote quantities, defined in the reference configuration with capital letters, in the current configuration with small letters and in the plastic intermediate configuration with a tilde. Upper indices $()^{\mathrm{e}}$, $()^{\mathrm{p}}$ denote elastic and plastic quantities respectively.

Green's strain tensor $\boldsymbol{E}$ in the reference configuration is given by

$$\begin{aligned}\boldsymbol{E} &= \frac{1}{2}\left(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{g}\boldsymbol{F} - \boldsymbol{G}\right) = \frac{1}{2}\left(\boldsymbol{F}^{\mathrm{pT}}\boldsymbol{F}^{\mathrm{eT}}\boldsymbol{g}\boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{p}} - \boldsymbol{G}\right) = \frac{1}{2}\left(\boldsymbol{F}^{\mathrm{pT}}\boldsymbol{F}^{\mathrm{eT}}\boldsymbol{g}\boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{p}} - \boldsymbol{F}^{\mathrm{pT}}\widetilde{\boldsymbol{G}}\boldsymbol{F}^{\mathrm{p}} + \boldsymbol{F}^{\mathrm{pT}}\widetilde{\boldsymbol{G}}\boldsymbol{F}^{\mathrm{p}} - \boldsymbol{G}\right) \\ &= \frac{1}{2}\boldsymbol{F}^{\mathrm{pT}}\left(\boldsymbol{F}^{\mathrm{eT}}\boldsymbol{g}\boldsymbol{F}^{\mathrm{e}} - \widetilde{\boldsymbol{G}}\right)\boldsymbol{F}^{\mathrm{p}} + \frac{1}{2}\left(\boldsymbol{F}^{\mathrm{pT}}\widetilde{\boldsymbol{G}}\boldsymbol{F}^{\mathrm{p}} - \boldsymbol{G}\right) = \frac{1}{2}(\boldsymbol{C} - \boldsymbol{C}^{\mathrm{p}}) + \frac{1}{2}(\boldsymbol{C}^{\mathrm{p}} - \boldsymbol{G}) = \boldsymbol{E}^{\mathrm{e}} + \boldsymbol{E}^{\mathrm{p}} \qquad (1)\end{aligned}$$

with metric tensors $\boldsymbol{g}$, $\widetilde{\boldsymbol{G}}$ and $\boldsymbol{G}$ in the current, the intermediate and the reference configurations respectively. It is obvious that Eq. (1) obtained using the multiplicative split of the deformation gradient is formally equivalent to the additive split of the strain tensor proposed by Green and Naghdi based on other constitutive assumptions.

Neither $\boldsymbol{E}^{\mathrm{e}}$ nor $\boldsymbol{E}^{\mathrm{p}}$ represent kinematic measures of physical strains. They should be calculated based on suitable constitutive assumptions. Additionally, due to the existence of both of the parts of the deformation gradient the elastic part of the strain tensor in the reference configuration does not describe a pure elastic material behavior. Certainly, after applying a plastic push-forward operation to $\boldsymbol{E}$ as well as to its parts, an additive split of the strain tensor can be obtained in the intermediate configuration:

$$\widetilde{\boldsymbol{E}} = \boldsymbol{F}^{\mathrm{p-T}}\boldsymbol{E}\boldsymbol{F}^{\mathrm{p-1}} = \frac{1}{2}(\widetilde{\boldsymbol{C}}^{\mathrm{e}} - \widetilde{\boldsymbol{G}}) + \frac{1}{2}(\widetilde{\boldsymbol{G}} - \widetilde{\boldsymbol{C}}^{\mathrm{p}}) = \widetilde{\boldsymbol{E}}^{\mathrm{e}} + \widetilde{\boldsymbol{E}}^{\mathrm{p}} \tag{2}$$

It should be mentioned that only in the reference configuration the elastic and plastic parts of the strain tensor represent pure elastic and plastic quantities (but again, not kinematic measures of real strains).

3. Principle laws of thermodynamics

Apart from the conservation laws of continuum mechanics which are valid independent of the special material behavior, deformation laws should be established guaranteeing their thermodynamical consistency – the observance of the first and second laws of thermodynamics.

The first law of thermodynamics describes the conservation of energy and is given in the local spatial description as follows:

$$\varrho\dot{\epsilon} = \boldsymbol{\sigma}\cdot\cdot\boldsymbol{d} - \operatorname{div}\boldsymbol{q} + \varrho h \tag{3}$$

with the contravariant Cauchy stress tensor $\boldsymbol{\sigma}$, the covariant tensor of the rate of deformation $\boldsymbol{d}$, the spatial mass density of the material ϱ, the internal energy density ϵ per unit mass, the heat flux vector $\boldsymbol{q}$ per unit area and a heat source density h per unit mass and per unit time. The second law of thermodynamics constitutes that the production of entropy is necessarily a non-negative quantity. Introducing the absolute temperature θ and the density of the entropy per unit mass η, this relation can be written in spatial local formulation as:

$$\varrho\dot{\eta} + \operatorname{div}\left(\frac{\boldsymbol{q}}{\theta}\right) - \varrho\frac{h}{\theta} \geqslant 0 \tag{4}$$

Defining the Helmholtz free energy density ψ per unit mass

$$\psi = \epsilon - \theta\eta \tag{5}$$

and combining the first and second laws of thermodynamics the well-known Clausius–Duhem inequality can be written:

$$-\varrho\left(\dot{\psi} + \dot{\theta}\eta\right) + \boldsymbol{\sigma}\cdot\cdot\boldsymbol{d} - \frac{1}{\theta}\boldsymbol{q}\operatorname{grad}\theta \geqslant 0 \tag{6}$$

with the simplified expression

$$-\varrho\dot{\psi} + \boldsymbol{\sigma}\cdot\cdot\boldsymbol{d} \geqslant 0 \tag{7}$$

in the isothermal case.

4. Some assumptions for a material model considering finite deformations

Apart from the well-established constitutive axioms (principles of determinism, equipresence, neighborhood, material frame indifference – see e.g. Narasimhan (1993)) we regard some other assumptions as useful to formulate a thermodynamically consistent deformation law for finite elasto-plastic deformations.

- Following the principle of covariance the deformation law is considered to be structure-invariant against mappings between the configurations. The covariance principle leads to the application of Lie-type derivatives of tensorial quantities in any configuration different from the reference one.
- The material model has been implemented into the experimental FEM-code PMHP based on the total-Lagrangean description. Accordingly, the deformation law will be defined in the reference configuration.
- The free energy density ψ is chosen in the reference configuration to be a function of the covariant material constitutive metric $\boldsymbol{C}$, a symmetric covariant tensor $\boldsymbol{C}^{\mathrm{p}}$ characterizing plastic deformations and a set of covariant deformation-like internal variables $\boldsymbol{A}_i$. We consider the following additive decomposition of the free energy density into an elastic part and a plastic part:
$$\psi = \psi(\boldsymbol{C}, \boldsymbol{C}^{\mathrm{p}}, \boldsymbol{A}_i) = \psi_{\mathrm{e}}(\boldsymbol{C}, \boldsymbol{C}^{\mathrm{p}}) + \psi_{\mathrm{p}}(\boldsymbol{A}_i) \tag{8}$$
- A physically correct definition of the hydrostatic stress state exists only in the current configuration. For this reason the invariants of the stress tensor and stress-like internal variables will be defined in the current configuration. In this case, we would emphasize that after the mapping of tensor invariants from the current to the reference configuration they should be formed using the metric tensor $\boldsymbol{C}$ instead of $\boldsymbol{G}$.
- The principle of conjugate variables which was originally postulated by Ziegler and McVean (1967) and Hill (1968) denotes the association of any stress tensor with a well-defined conjugate strain tensor independent on the special material behavior. If the scalar stress power per unit mass of a body is defined in the current configuration as (see Eq. (3))
$$\frac{1}{\varrho}\boldsymbol{\sigma} \cdot\cdot\, \boldsymbol{d} \tag{9}$$
it should remain at the same value after a mapping of the stress tensor and the tensor of the rate of deformation to the reference configuration:
$$\frac{1}{\varrho}\boldsymbol{\sigma} \cdot\cdot\, \boldsymbol{d} = \frac{1}{\varrho_0}\boldsymbol{\tau} \cdot\cdot\, \boldsymbol{d} = \frac{1}{\varrho_0}\left(\boldsymbol{F}\boldsymbol{T}\boldsymbol{F}^{\mathrm{T}}\right) \cdot\cdot\, (\boldsymbol{F}^{-\mathrm{T}}\overset{\bullet}{\boldsymbol{E}}\boldsymbol{F}^{-1}) = \frac{1}{\varrho_0}\boldsymbol{T} \cdot\cdot\, \overset{\bullet}{\boldsymbol{E}} \tag{10}$$
with the contravariant second Piola–Kirchhoff stress tensor $\boldsymbol{T}$, the contravariant Kirchhoff stress tensor $\boldsymbol{\tau}$ and the mass density in the reference configuration ϱ_0.
The concept of dual variables was postulated by Haupt and Tsakmakis (1989). It defines pairs of stress and strain tensors in such a way that apart from the stress power also the conjugate stress power as well as the incremental stress power are invariant under a group of transformations corresponding to a set of physically reasonable intermediate configurations.
We introduce an arbitrary linear mapping $\boldsymbol{F}^{\star}$ of tangential spaces in material points of the reference configuration to tangential spaces of an arbitrary intermediate configuration. In the special case of the mapping to the current configuration we obtain $\boldsymbol{F}^{\star} = \boldsymbol{F}$. Considering the concept of dual variables the stress power and the incremental stress power per unit mass of a body will be mapped between the reference configuration and an arbitrary configuration denoted by $\hat{()}$ using push-forward and pull-back operations with respect to $\boldsymbol{F}^{\star}$:
$$\frac{1}{\varrho_0}\boldsymbol{T} \cdot\cdot\, \overset{\bullet}{\boldsymbol{E}} = \frac{1}{\varrho_0}\left(\boldsymbol{F}^{\star^{-1}}\hat{\boldsymbol{\tau}}\boldsymbol{F}^{\star^{-\mathrm{T}}}\right) \cdot\cdot\, \left(\boldsymbol{F}^{\star^{\mathrm{T}}}\overset{\triangle}{\hat{\boldsymbol{e}}}\boldsymbol{F}^{\star}\right) = \frac{1}{\varrho_0}\hat{\boldsymbol{\tau}} \cdot\cdot\, \overset{\triangle}{\hat{\boldsymbol{e}}} \tag{11}$$

$$\frac{1}{\varrho_0}\overset{\bullet}{\boldsymbol{T}}\cdot\cdot\overset{\bullet}{\boldsymbol{E}} = \frac{1}{\varrho_0}\left(\boldsymbol{F}^{\star^{-1}}\overset{\triangledown}{\hat{\boldsymbol{\tau}}}\boldsymbol{F}^{\star^{-\mathrm{T}}}\right)\cdot\cdot\left(\boldsymbol{F}^{\star^{\mathrm{T}}}\overset{\triangle}{\hat{\boldsymbol{e}}}\boldsymbol{F}^{\star}\right) = \frac{1}{\varrho_0}\overset{\triangledown}{\hat{\boldsymbol{\tau}}}\cdot\cdot\overset{\triangle}{\hat{\boldsymbol{e}}} \tag{12}$$

5. Basic relations of a thermodynamically consistent deformation law for finite elasto-plastic deformations

Considering the concept of conjugate variables and applying pull-back operations to relation (7), the Clausius–Duhem inequality for isothermal deformations in the reference configuration is known as

$$-\varrho_0\dot{\psi} + \frac{1}{2}\boldsymbol{T}\cdot\cdot\dot{\boldsymbol{C}} \geqslant 0 \tag{13}$$

Based on the additive split of the free energy density (8) we propose its following special representation

$$\psi = \psi_{\mathrm{e}}\left(\frac{1}{2}(\boldsymbol{C} - \boldsymbol{C}^{\mathrm{p}})\right) + \psi_{\mathrm{p}}(\boldsymbol{A}_1) = \psi_{\mathrm{e}}(\boldsymbol{E}^{\mathrm{e}}) + \psi_{\mathrm{p}}(\boldsymbol{A}_1) \tag{14}$$

introducing a covariant symmetric second-order tensorial internal variable $\boldsymbol{A}_1$ which is considered to be work-conjugate to the backstress tensor. The following relation is obtained for the inequality (13) using the special formulation (14) of the free energy density:

$$-\rho_0\left\{\frac{\partial\psi_{\mathrm{e}}}{\partial\boldsymbol{E}^{\mathrm{e}}}\cdot\cdot\dot{\boldsymbol{E}}^{\mathrm{e}} + \frac{\partial\psi_{\mathrm{p}}}{\partial\boldsymbol{A}_1}\cdot\cdot\dot{\boldsymbol{A}}_1\right\} + \boldsymbol{T}\cdot\cdot\left(\dot{\boldsymbol{E}}^{\mathrm{e}} + \frac{1}{2}\dot{\boldsymbol{C}}^{\mathrm{p}}\right) \geqslant 0 \tag{15}$$

As in case of pure elastic material behavior no dissipation does appear, the elimination of a hyperelastic deformation law

$$\boldsymbol{T} = \rho_0\frac{\partial\psi_{\mathrm{e}}}{\partial\boldsymbol{E}^{\mathrm{e}}} = \frac{\partial(\rho_0\psi_{\mathrm{e}})}{\partial\boldsymbol{E}^{\mathrm{e}}} = \frac{\partial\bar{\psi}_{\mathrm{e}}}{\partial\boldsymbol{E}^{\mathrm{e}}} \tag{16}$$

to characterize the elastic part of the material behavior does not violate the inequality (15). Assuming for the backstress tensor $\boldsymbol{\alpha}$

$$\boldsymbol{\alpha} = \rho_0\frac{\partial\psi_{\mathrm{p}}}{\partial\boldsymbol{A}_1} = \frac{\partial\bar{\psi}_{\mathrm{p}}}{\partial\boldsymbol{A}_1} \tag{17}$$

and considering Eq. (16), the remaining part of the Clausius–Duhem inequality (15) constitutes the inequality of the plastic dissipation

$$\mathscr{D}^{\mathrm{p}} = -\boldsymbol{\alpha}\cdot\cdot\dot{\boldsymbol{A}}_1 + \frac{1}{2}\boldsymbol{T}\cdot\cdot\dot{\boldsymbol{C}}^{\mathrm{p}} \geqslant 0 \tag{18}$$

The plastic dissipation has to achieve a maximum under the constraint of satisfying an appropriate yield condition $F(\boldsymbol{T},\boldsymbol{\alpha}) = 0$ (see e.g. Simo (1988)).

A corresponding constrained optimization problem based on the method of Lagrange multipliers (here λ represents the plastic multiplier) is defined as follows:

$$\mathscr{M} = \mathscr{D}^{\mathrm{p}}(\boldsymbol{T},\boldsymbol{\alpha}) - \lambda F(\boldsymbol{T},\boldsymbol{\alpha}) \quad \rightarrow \quad \max \tag{19}$$

Finally, solving the following system of equations representing necessary conditions (Kuhn–Tucker conditions) for the objective function $\mathscr{M}$ to be a maximum

$$\frac{\partial\mathscr{M}}{\partial\boldsymbol{T}} = \frac{\partial\mathscr{D}^{\mathrm{p}}(\boldsymbol{T},\boldsymbol{\alpha})}{\partial\boldsymbol{T}} - \lambda\frac{\partial F(\boldsymbol{T},\boldsymbol{\alpha})}{\partial\boldsymbol{T}} = \boldsymbol{0} \tag{20}$$

$$\frac{\partial \mathscr{M}}{\partial \boldsymbol{\alpha}} = \frac{\partial \mathscr{D}^{\mathrm{p}}(\boldsymbol{T}, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} - \lambda \frac{\partial F(\boldsymbol{T}, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} = \mathbf{0} \tag{21}$$

we obtain the evolutional equations for the internal variables in a generalized formulation:

$$2\dot{\boldsymbol{E}}^{\mathrm{p}} = \dot{\boldsymbol{C}}^{\mathrm{p}} = 2\lambda \frac{\partial F}{\partial \boldsymbol{T}}, \qquad \dot{\boldsymbol{A}}_1 = -\lambda \frac{\partial F}{\partial \boldsymbol{\alpha}} \tag{22}$$

Apart from the fulfilling of the necessary conditions of the maximum of $\mathscr{M}$ the validity of the inequality (18) for arbitrary stress and strain states should be proved in case of each special deformation law.

Based on Eq. (16) the rate formulation of the stress tensor is given by

$$\dot{\boldsymbol{T}} = \underset{4}{\boldsymbol{D}} \cdot \cdot \dot{\boldsymbol{E}}^{\mathrm{e}} \text{ with the contravariant tensor } \underset{4}{\boldsymbol{D}} = \frac{\partial^2 \bar{\psi}_{\mathrm{e}}}{\partial \boldsymbol{E}^{\mathrm{e}} \partial \boldsymbol{E}^{\mathrm{e}}} \tag{23}$$

Due to the dependency of the yield function on the equivalent stress T_F which on its part represents a function of the plastic arc length $E^{\mathrm{p}}_{\mathrm{v}}$ it is necessary to consider an evolutional equation for $E^{\mathrm{p}}_{\mathrm{v}}$. Following the usual representation we assume

$$\dot{E}^{\mathrm{p}}_{\mathrm{v}} = \sqrt{\tfrac{2}{3} \boldsymbol{B} \dot{\boldsymbol{E}}^{\mathrm{p}} \cdot \cdot \boldsymbol{B} \dot{\boldsymbol{E}}^{\mathrm{p}}} \tag{24}$$

with $\boldsymbol{B} = \boldsymbol{C}^{-1}$.

It can be numerically shown that the updating of stress increments based on a time discretization of Eq. (23) diverges from the stress solution based on Eq. (16). To avoid unjustified differences of the calculated stresses from the real values induced by the algorithm we propose the following deformation law for elasto-plastic material behavior as a system of differential and algebraic equations considering Eqs. (22) and (24):

$$\dot{\boldsymbol{C}}^{\mathrm{p}} - 2\lambda \frac{\partial F}{\partial \boldsymbol{T}} = \mathbf{0} \tag{25}$$

$$\dot{\boldsymbol{\alpha}} + \lambda \boldsymbol{Q}_1(\boldsymbol{T}, \boldsymbol{\alpha}, \boldsymbol{p}) = \mathbf{0} \tag{26}$$

$$\dot{E}^{\mathrm{p}}_{\mathrm{v}} + \lambda Q_2(\boldsymbol{T}, \boldsymbol{\alpha}, \boldsymbol{p}) = 0 \tag{27}$$

$$F(\boldsymbol{T}, \boldsymbol{\alpha}, \boldsymbol{p}) = 0 \tag{28}$$

with the material parameters $\boldsymbol{p} = (p_1, \ldots, p_{np})^{\mathrm{T}}$ characterizing the hardening behavior and

$$\boldsymbol{Q}_1 = \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{A}_1} \cdot \cdot \frac{\partial F}{\partial \boldsymbol{\alpha}}, \quad Q_2 = -\sqrt{\frac{2}{3} \boldsymbol{B} \frac{\partial F}{\partial \boldsymbol{T}} \cdot \cdot \boldsymbol{B} \frac{\partial F}{\partial \boldsymbol{T}}} \tag{29}$$

6. Formulation of a special deformation law

Describing the material behavior of metals we propose the following modified compressible Neo-Hookean model for the elastic part of the free energy density:

$$\bar{\psi}_{\mathrm{e}} = c_{10}\Big(I(\check{\boldsymbol{C}}) - \ln III(\check{\boldsymbol{C}}) - 3\Big) + D_2\Big(\ln III(\check{\boldsymbol{C}})\Big)^2 \tag{30}$$

with the material parameters c_{10}, D_2 which can be estimated based on the Young's modulus and the Poisson's ratio. Furthermore, we introduced the modified covariant strain tensor

$$\check{\boldsymbol{C}} = \boldsymbol{C} - \boldsymbol{C}^{\mathrm{p}} + \boldsymbol{G} = 2\boldsymbol{E}^{\mathrm{e}} + \boldsymbol{G} \tag{31}$$

We suggest a yield condition formulated with the deviatoric parts of the stress and the backstress tensors

$$F = (\grave{\boldsymbol{T}} - \grave{\boldsymbol{\alpha}}) \cdot\cdot \underset{4}{\boldsymbol{K}} \cdot\cdot \left(\grave{\boldsymbol{T}} - \grave{\boldsymbol{\alpha}}\right) - \tfrac{2}{3}T_F^2 = 0 \tag{32}$$

with

$$\grave{\boldsymbol{T}} = \boldsymbol{T} - \tfrac{1}{3}(\boldsymbol{T} \cdot\cdot \boldsymbol{C})\boldsymbol{B} \tag{33}$$

and the yield stress T_F. Relation (32) is similar to a yield condition proposed by Baltov and Sawczuk (1965) for small elasto-plastic deformations. The fourth-order covariant tensor $\underset{4}{\boldsymbol{K}}$ describing the distorsional hardening consists of an isotropic part $\underset{4}{\boldsymbol{K}}^{\mathrm{i}}$ and an anisotropic part $\underset{4}{\boldsymbol{K}}^{\mathrm{a}}$

$$\underset{4}{\boldsymbol{K}} = \underset{4}{\boldsymbol{K}}^{\mathrm{i}} + \underset{4}{\boldsymbol{K}}^{\mathrm{a}} \tag{34}$$

with

$$K^{\mathrm{i}}_{IJKL} = \tfrac{1}{2}\left(C_{IK}C_{JL} + C_{IL}C_{JK} - \tfrac{2}{3}C_{IJ}C_{KL}\right) \tag{35}$$

At the current stage of our investigations the evolution of the anisotropic part of this fourth-order tensor is neglected, but an initial anisotropy of the material can be considered.

To calculate the yield stress T_F in dependency of the plastic arc length $E^{\mathrm{p}}_{\mathrm{v}}$ we suggest a power law

$$T_F = T_{F_0} + a\left[\left(E^{\mathrm{p}}_{\mathrm{v}} + \beta\right)^n - \beta^n\right] \tag{36}$$

with the material parameters T_{F_0} (initial yield stress), a, n. Furthermore, the parameter β is introduced to avoid infinite derivatives of Eq. (36) with respect to the plastic arc length in the case $E^{\mathrm{p}}_{\mathrm{v}} = 0$.

Suggesting the following simple formulation for the plastic part of the free energy density

$$\bar{\psi}_{\mathrm{p}}(\boldsymbol{A}_1) = \tfrac{1}{2}c\boldsymbol{A}_1\boldsymbol{G} \cdot\cdot \boldsymbol{A}_1\boldsymbol{G} \tag{37}$$

with the material parameter c we obtain after some transformations based on the relations (17), (29), (32) and (36) the following special formulation for the evolutional functions $\boldsymbol{Q}_1$ and Q_2:

$$\boldsymbol{Q}_1 = -2c\boldsymbol{G}\left[\underset{4}{\boldsymbol{K}} \cdot\cdot (\grave{\boldsymbol{T}} - \grave{\boldsymbol{\alpha}})\right]\boldsymbol{G} \tag{38}$$

$$Q_2 = -2\sqrt{\tfrac{2}{3}(\grave{\boldsymbol{T}} - \grave{\boldsymbol{\alpha}}) \cdot\cdot \underset{4}{\boldsymbol{K}} \cdot\cdot (\grave{\boldsymbol{T}} - \grave{\boldsymbol{\alpha}})} \tag{39}$$

It can be easily shown that the plastic dissipation inequality

$$\mathscr{D}^{\mathrm{p}} = -\rho_0 \frac{\partial\psi_{\mathrm{p}}}{\partial \boldsymbol{A}_1} \cdot\cdot \dot{\boldsymbol{A}}_1 + \frac{1}{2}\boldsymbol{T} \cdot\cdot \dot{\boldsymbol{C}}^{\mathrm{p}} \geqslant 0 \tag{40}$$

based on the relations (29), (32) and (36) is fulfilled.

7. An implicit algorithm to integrate the deformation law given in rate formulation

Within the framework of a finite element algorithm the DAE-system (25)–(28) with the proposed constitutive equations (32), (38) and (39) has to be integrated at each load step in each integration point of the FE-mesh to calculate the increments of $\boldsymbol{C}^{\mathrm{p}}$, the internal variables describing the hardening behavior and the plastic multiplier. For this reason the differential equations are discretized in time using the following generalized implicit one-step iteration scheme

$$y_{n+1} = y_n + (\gamma f_{n+1} + (1-\gamma) f_n)\Delta t \tag{41}$$

with

$$\Delta t = t_{n+1} - t_n \tag{42}$$

for the numerical solution of an ordinary differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \dot{y} = f(t, y) \tag{43}$$

The parameter $\gamma \in [0,1]$ can be chosen freely and it controls the velocity of the convergency of the solution. The case $\gamma = 1$ is well known as the Euler backward scheme, the case $\gamma = 0.5$ is named the Crank–Nicolson method or the trapezium rule.

The time discretization of the DAE-system (25)–(27) based on the relation (41) results in the following system of nonlinear algebraic equations with respect to the increments of $\boldsymbol{C}^{\mathrm{p}}$, the internal variables describing the hardening behavior and the plastic multiplier completed by the algebraic constraint (28):

$$\boldsymbol{C}^{\mathrm{p}j}_{n+1} - \boldsymbol{C}^{\mathrm{p}}_n - 2\left[\gamma\lambda^j_{n+1}\left.\frac{\partial F}{\partial \boldsymbol{T}}\right|^j_{n+1} + (1-\gamma)\lambda_n\left.\frac{\partial F}{\partial \boldsymbol{T}}\right|_n\right]\Delta t = \boldsymbol{0} \tag{44}$$

$$\boldsymbol{\alpha}^j_{n+1} - \boldsymbol{\alpha}_n + \left[\gamma\lambda^j_{n+1}(\boldsymbol{Q}_1)^j_{n+1} + (1-\gamma)\lambda_n(\boldsymbol{Q}_1)_n\right]\Delta t = \boldsymbol{0} \tag{45}$$

$$\left(E^{\mathrm{p}}_{\mathrm{v}}\right)^j_{n+1} - \left(E^{\mathrm{p}}_{\mathrm{v}}\right)_n + \left[\gamma\lambda^j_{n+1}(Q_2)^j_{n+1} + (1-\gamma)\lambda_n(Q_2)_n\right]\Delta t = 0 \tag{46}$$

$$F(\boldsymbol{T}^j_{n+1}, \boldsymbol{\alpha}^j_{n+1}) = 0 \tag{47}$$

The upper index j denotes the jth step of a Newton's algorithm to achieve the equilibrium during the current load increment $[t_n, t_{n+1}]$ indicated by the lower index n.

For simplicity, defining an operator $\boldsymbol{G}(\boldsymbol{z}_n, \boldsymbol{z}^j_{n+1})$ and a vector $\boldsymbol{z} = (\boldsymbol{C}^{\mathrm{p}}, \boldsymbol{\alpha}, E^{\mathrm{p}}_{\mathrm{v}}, \lambda)^{\mathrm{T}}$, the system (44)–(47) can be written in the more compact form

$$\boldsymbol{G}^j_{n+1} = \boldsymbol{G}(\boldsymbol{z}_n, \boldsymbol{z}^j_{n+1}) = \boldsymbol{0} \tag{48}$$

with the vector $\boldsymbol{z}^j_{n+1} = (\boldsymbol{C}^{\mathrm{p}j}_{n+1}, \boldsymbol{\alpha}^j_{n+1}, (E^{\mathrm{p}}_{\mathrm{v}})^j_{n+1}, \lambda^j_{n+1})^{\mathrm{T}}$ of unknown variables. Based on a representation of Eq. (48) as a Taylor's series in the neighbourhood of a given iterative solution $(\boldsymbol{z}^j_{n+1})^i$ considering only linear terms

$$\left(\boldsymbol{G}^j_{n+1}\right)^i + \left[\boldsymbol{\nabla}_{\left(\boldsymbol{z}^j_{n+1}\right)^i}\boldsymbol{G}\right]\left[\left(\boldsymbol{z}^j_{n+1}\right)^{i+1} - \left(\boldsymbol{z}^j_{n+1}\right)^i\right] = \boldsymbol{0} \tag{49}$$

we obtain a Newton's method for the solution $\left(\boldsymbol{z}^j_{n+1}\right)^{i+1}$ of the system of nonlinear algebraic equations (48). Each iteration process to solve the system (44)–(47) starts with an elastic predictor

$$\left(\boldsymbol{T}^j_{n+1}\right)^0 = \left.\frac{\partial\bar{\psi}_{\mathrm{e}}}{\partial \boldsymbol{E}^{\mathrm{e}}}\right|_{\boldsymbol{C}^j_{n+1}, \boldsymbol{C}^{\mathrm{p}}_n} \tag{50}$$

In case of

$$F\left(\left(\boldsymbol{T}_{n+1}^{j}\right)^{0},\boldsymbol{\alpha}_{n}\right)<0 \tag{51}$$

pure elastic material behavior is obtained, and the internal variables remain unchanged for this equilibrium state. On the other hand, if the predictor state violates the constraint condition (51), we start an iterative plastic process in the sense of a generalized return algorithm with the following initial values given at the beginning of the time step $[t_n, t_{n+1}]$:

$$\left(z_{n+1}^{j}\right)^{0}=\left(\boldsymbol{C}_{n}^{\mathrm{p}},\boldsymbol{\alpha}_{n},\left(E_{\mathrm{v}}^{\mathrm{p}}\right)_{n},\lambda_{n}\right)^{\mathrm{T}} \tag{52}$$

Finally, the calculation of $\boldsymbol{C}^{\mathrm{p}}$, the internal variables and the plastic multiplier results in the solution of the system of linear algebraic equations (49) at each iteration of the local Newton's process to integrate the deformation law (which is embedded in the global Newton's process to fulfill the equilibrium of inner and outer forces) with the Jacobian matrix $\nabla_z \boldsymbol{G}$ and the right-hand side $-\boldsymbol{G}$. At each step i of the local iterative procedure the stress tensor will be updated using the expression

$$\left(\boldsymbol{T}_{n+1}^{j}\right)^{i}=\left.\frac{\partial\bar{\psi}_{\mathrm{e}}}{\partial\boldsymbol{E}^{\mathrm{e}}}\right|_{\boldsymbol{C}_{n+1}^{j},\left(\boldsymbol{C}_{n+1}^{\mathrm{p}j}\right)^{i}} \tag{53}$$

As shown by Görke et al. (2000) in case of the concrete basic model for the FE-code PMHP, the rate formulation of the principle of virtual work (the incremental weak formulation of the equilibrium)

$$\int_{V_0}\left\{\left(\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}\boldsymbol{E}}\cdot\cdot\dot{\boldsymbol{E}}\right)\cdot\cdot\delta\dot{\boldsymbol{E}}+\boldsymbol{T}\cdot\cdot\left[\left(\operatorname{grad}(\dot{\boldsymbol{U}})\right)^{\mathrm{T}}\operatorname{grad}(\delta\dot{\boldsymbol{U}})\right]\right\}\mathrm{d}V_0=\int_{\delta V_0}\dot{\boldsymbol{R}}\delta\dot{\boldsymbol{U}}\,\mathrm{d}(\delta V_0)+\int_{V_0}\varrho_0\dot{\boldsymbol{K}}\,\delta\dot{\boldsymbol{U}}\,\mathrm{d}V_0 \tag{54}$$

with surface and mass forces $\boldsymbol{R}$ and $\boldsymbol{K}$ respectively and the displacement vector $\boldsymbol{U}$ contains the material matrix $\mathrm{d}\boldsymbol{T}/\mathrm{d}\boldsymbol{E}$. To achieve quadratic convergency solving the linearized boundary value problem for the equilibrium using a Netwon–Raphson method the material matrix should be consistent to the embedded stress algorithm (initial value problem).

One of the most important advantages of the presented method of an implicit integration of the deformation law consists in the efficient determination of the consistent material matrix in its most general form. With this aim in view we perform an implicit differentiation of the system of non-linear equations (48) at the end of the local iteration procedure for the deformation law with respect to the total strain tensor

$$\frac{\mathrm{d}\boldsymbol{G}}{\mathrm{d}\boldsymbol{E}_{n+1}^{j}}=\frac{\partial\boldsymbol{G}}{\partial\boldsymbol{E}_{n+1}^{j}}+\left(\nabla_{z_{n+1}^{j}}\boldsymbol{G}\right)\frac{\mathrm{d}z_{n+1}^{j}}{\mathrm{d}\boldsymbol{E}_{n+1}^{j}}=\boldsymbol{0} \tag{55}$$

It can be shown that the trivial solution

$$\frac{\mathrm{d}\boldsymbol{C}^{\mathrm{p}}}{\mathrm{d}\boldsymbol{E}}=\underset{4}{\boldsymbol{0}} \tag{56}$$

represents the only solution of the system (55). Considering Eqs. (1) and (23) we get

$$\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}\boldsymbol{E}}=\frac{1}{2}\underset{4}{\boldsymbol{D}}\cdot\cdot\left(\frac{\mathrm{d}\boldsymbol{C}}{\mathrm{d}\boldsymbol{E}}-\frac{\mathrm{d}\boldsymbol{C}^{\mathrm{p}}}{\mathrm{d}\boldsymbol{E}}\right)=\underset{4}{\boldsymbol{D}}\cdot\cdot\left(\underset{4}{\boldsymbol{I}}-\frac{1}{2}\frac{\mathrm{d}\boldsymbol{C}^{\mathrm{p}}}{\mathrm{d}\boldsymbol{E}}\right). \tag{57}$$

Therefore, it is obvious that in case of the presented stress algorithm the consistent material matrix represents the hyperelastic matrix defined by Eq. (23).

8. Numerical example

An infinitely long plane-strain strip with quadratic cross-section (edge length 1 mm) and a circular hole in the centre (diameter 0.2 mm) is subjected to vertical displacements. For symmetry reasons, only one quarter of the strip is considered. The FE-mesh employed is shown in Fig. 1 as well as its distribution to the different processors of a parallel computer. Due to the natural parallelism of the local stress algorithm and the assembly of the stiffness matrix, their speed-up at the parallel computer is nearly an optimal one. Otherwise, the speed-up of the entire FE-solution essentially depends on the share of communication time between the processors required for input and output processes as well as for the solution of the global stiffness system.

The material parameters for the Neo-Hookean model of the elastic part of the free energy density (30) are estimated based on a Young's modulus $E = 210$ GPa and a Poisson's ratio $v = 0.3$. The values for the hardening parameters in Eqs. (36) and (37) are $c = 500$ MPa, $T_{F_0} = 200$ MPa, $a = 1000$ MPa, $n = 0.3$ and $\beta = 0.0001$. Both isotropic and kinematic hardening with initial isotropy are considered.

The displacements are increased linearly until an extension of 100% with respect to the undeformed state. Fig. 2 shows the development of the value of the plastic arc length representing the plastification process at different load levels. To plot these results, the plastic arc length computed at the Gauss points is projected onto the nodes of the FE-mesh by the interpolation functions of the elements. The plastification starts near the hole at point B (see Fig. 1), and the plastic arc length attains a value of 1.1 at the maximum vertical displacement. In a region about point A near the hole an unyielded area remains even at the maximum load.

Applying the maximum boundary displacements in 100 load steps, the global Newton solution strategy converges within 3–6 iterations at each load step, and the number of local iterations does not exceed 12. If the calculation is completed successfully with 30 load steps performing 4–8 global iterations at each load

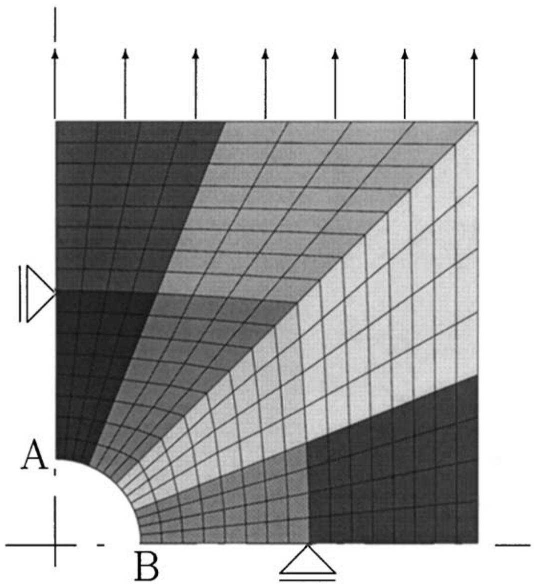

Fig. 1. Plane-strain strip with hole (one quarter of the cross-section). Distribution of the FE-mesh on eight processors and schematic presentation of the boundary conditions.

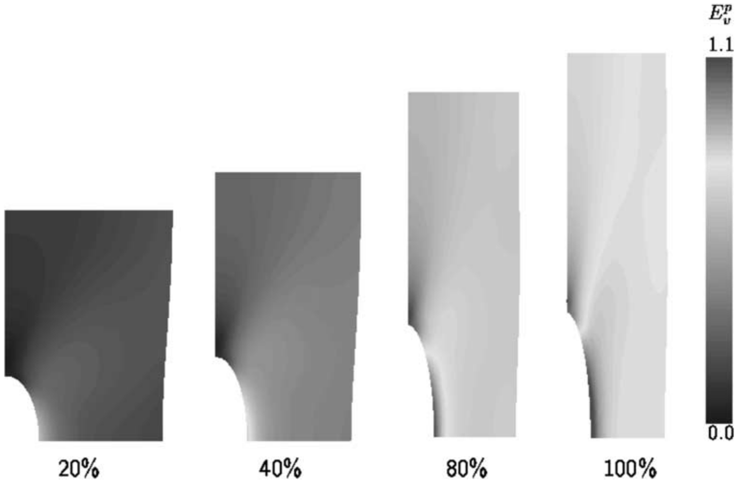

Fig. 2. Plane-strain strip with hole. Development of the plastic arc length at different load levels. Presentation of the deformed geometry in real scale. Vertical displacement of the top boundary 20%, 40%, 80% and 100% of the height of the undeformed strip respectively.

step and maximum 14 local iterations, the global iterative procedure diverges for a lower number of load steps.

The numerical simulation is performed on a parallel computer with eight processors using the nonlinear experimental FE-code PMHP developed at the Chemnitz University of Technology. A coarse grid with eight-node quadrilateral elements with biquadratic isoparametric form functions is introduced, and will be internally subdivided twice. Convergency of the global and local Newton procedures are measured in terms of the Euclidean norm of the corresponding residual vectors. If the global stiffness system is solved by a parallel preconditioned conjugated gradient method, for the solution of local systems of linear algebraic equations like Eq. (49) a direct method with the selection of pivote elements is applied.

9. Semianalytical sensitivity analysis

The proposed method of the identification of material parameters analyzing inhomogeneous displacement fields using gradient-based nonlinear optimization procedures is explained in detail in Bohnsack (1997) and Görke and Kreißig (1997) for the case of small elasto-plastic deformations. Some important aspects regarding their application to the case of finite deformations will be presented shortly.

The basic idea is the minimization of the following least-squares type objective function $\Phi \rightarrow \min\limits_{\boldsymbol{p}}$:

$$\Phi(\boldsymbol{p}) = \frac{1}{2} \sum_{i=1}^{n_L} \sum_{j=1}^{n_T} \sum_{K=1}^{3} \left(\{U_K(\boldsymbol{p})\}_{ij} - \{\bar{U}_K\}_{ij} \right)^2 \tag{58}$$

with the calculated coordinates of the displacement vector U_K and the measured ones $\bar{U}_K$. Using the FEM for the calculation of the comparative values of the displacements, the variables $U_K(\boldsymbol{p})$ represent the nodal displacements depending on the material parameters $\boldsymbol{p}$ and detected in n_T measurement points for n_L load steps. Within the framework of gradient-based optimization methods an improved set of the material parameters $\boldsymbol{p}_{l+1}$ can be obtained using the following iterative procedure:

$$\boldsymbol{p}_{l+1} = \boldsymbol{p}_l - \omega \boldsymbol{Y}_l^{-1} \nabla \Phi_l \tag{59}$$

with the search step length ω. The search direction is characterized by the gradient of the objective function

$$\nabla \Phi_l = \sum_{i=1}^{n_L} \sum_{j=1}^{n_T} \sum_{K=1}^{3} \left(\{U_K(\boldsymbol{p}_l)\}_{ij} - \left\{\bar{U}_K\right\}_{ij} \right) \frac{\mathrm{d}\{U_K\}_{ij}}{\mathrm{d}\boldsymbol{p}_l} \tag{60}$$

and a suitable matrix $\boldsymbol{Y}_l$ affecting the convergency speed of the iterative algorithm (59) (e.g. in case of the method of steepest descent $\boldsymbol{Y}_l = \boldsymbol{I}$).

Based on a proposal of Mahnken and Stein (1997) it can be shown that the derivation of the balance law of linear momentum with respect to a material parameter p results in a weak formulation similar to the rate formulation of the global equilibrium. Following, a stiffness system for the calculation of the derivatives of the nodal displacements with respect to a material parameter – known as sensitivity analysis – can be obtained within the framework of a finite element procedure:

$$\boldsymbol{K}_T \frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}p} = \boldsymbol{P}_p \tag{61}$$

with

$$\boldsymbol{P}_p = \biguplus_{e=1}^{\mathrm{numel}} \boldsymbol{P}_p^e \quad \text{and} \quad \boldsymbol{P}_p^e = -\int_{V_0^e} \boldsymbol{B}^{\mathrm{T}} \frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}p} \mathrm{d}V_0^e \tag{62}$$

The system (61) is similar to the stiffness system for the finite element boundary value problem with the known global stiffness matrix $\boldsymbol{K}_T$. The right-hand side of Eq. (61) contains derivatives of the stress tensor with respect to a material parameter $\mathrm{d}\boldsymbol{T}/\mathrm{d}p$. They can be obtained considering the dependency of the discretized deformation law (48) on the material parameters

$$\boldsymbol{G}(\boldsymbol{z}_n(\boldsymbol{p}), \boldsymbol{z}_{n+1}(\boldsymbol{p}), \boldsymbol{p}) = \boldsymbol{0} \tag{63}$$

After an implicit differentiation of Eq. (63) with respect to a material parameter we get the following relation:

$$\frac{\mathrm{d}\boldsymbol{G}_{n+1}}{\mathrm{d}p} = \frac{\partial \boldsymbol{G}_{n+1}}{\partial \boldsymbol{z}_n} \frac{\mathrm{d}\boldsymbol{z}_n}{\mathrm{d}p} + \frac{\partial \boldsymbol{G}_{n+1}}{\partial \boldsymbol{z}_{n+1}} \frac{\mathrm{d}\boldsymbol{z}_{n+1}}{\mathrm{d}p} + \frac{\partial \boldsymbol{G}_{n+1}}{\partial p} = \boldsymbol{0} \tag{64}$$

or

$$\left(\nabla_{\boldsymbol{z}_{n+1}} \boldsymbol{G}\right) \frac{\mathrm{d}\boldsymbol{z}_{n+1}}{\mathrm{d}p} = -\frac{\partial \boldsymbol{G}_{n+1}}{\partial \boldsymbol{z}_n} \frac{\mathrm{d}\boldsymbol{z}_n}{\mathrm{d}p} - \frac{\partial \boldsymbol{G}_{n+1}}{\partial p} \tag{65}$$

Again, Eq. (65) represents a system of linear algebraic equations with the known Jacobian matrix $\nabla_{\boldsymbol{z}} \boldsymbol{G}$ and the right-hand side consisting of likewise known expressions. Using a direct method to solve system (49), the derivatives $\mathrm{d}\boldsymbol{C}^{\mathrm{p}}/\mathrm{d}p$ as a part of $\mathrm{d}\boldsymbol{z}_{n+1}/\mathrm{d}p$ can be easily obtained multiplying the right-hand side of the system (65) by the inverted Jacobian matrix. Performing the differentiation of the Eq. (16) with respect to a material parameter p we get a relation between the required derivatives $\mathrm{d}\boldsymbol{T}/\mathrm{d}p$ and the obtained values of $\mathrm{d}\boldsymbol{C}^{\mathrm{p}}/\mathrm{d}p$.

$$\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}p} = -\frac{1}{2} \underset{4}{\boldsymbol{D}} \cdot\cdot \frac{\mathrm{d}\boldsymbol{C}^{\mathrm{p}}}{\mathrm{d}p} \tag{66}$$

The presented algorithm of the determination of the gradient of the objective function is called semi-analytical sensitivity analysis, and distinguishes from pure analytical or numerical methods by its high efficiency and accuracy. It should be carried out for each material parameter p_i of the parameter vector $\boldsymbol{p}$.

10. Conclusions

The object of our investigations is the identification of material parameters for finite elasto-plastic deformations analyzing inhomogeneous displacement fields based on nonlinear optimization procedures. The numerical values of the quantities to be compared with measurements are calculated using the finite element method.

In this paper the attempt of a generalization of existing theoretical material models suitable for the purpose of the parameter identification has been presented. The objective was to conserve a most general structure of the deformation law as a system of differential and algebraic equations independent of special formulations for the yield function and the evolutional equations. Our approach is based on the consistent application of the concept of dual variables, the covariance principle and some other physical useful and convenient assumptions. We presented the basic relations of a thermodynamically consistent material model for finite elasto-plastic deformations in the isothermal case. They provide some assumptions for suitable special formulations of the free energy density, the yield condition and the evolutional equations for internal variables.

We adapted and modified basic implicit algorithms for the computation of stresses and internal variables distinguishing oneself by their high efficiency. The consistency of the computation of the material matrix and of the semianalytical sensitivity analysis with respect to the stress algorithm has been shown.

A generalized programme interface serving the presented material model has been successfully realized in the experimental FE-code PMHP as well as the numerical algorithms for the computation of stresses, internal variables and the consistent material matrix. PMHP is based on a total-Lagrangean description and has been adapted to parallel computers. A numerical example using a deformation law considering isotropic and kinematic hardening has been presented.

Future investigations concern the verification of the different formulations of the deformation law for finite elasto-plastic deformations on experimental results, and the review of their suitability in the process of the parameter identification.

Acknowledgements

This study was partly funded by the DFG. The authors acknowledge helpful discussion with Prof. P. Haupt.

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