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Local and global analysis of inhomogeneous displacement fields for the identification of material parameters

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Abstract

The inverse problem of the identification of material parameters has been solved, using nonlinear deterministic optimization methods with semianalytical sensitivity analysis based on the implicit differentiation of the equilibrium conditions and the deformation law. An indirect analysis of displacements at exposed positions of a specimen, using the local integration of the deformation law, and the direct analysis of the entire displacement fields, using the Finite Element Method, are joined for the solution of the direct problem to be solved at each optimization step. The successful application of the complex method is demonstrated on the identification of the material parameters of a special steel alloy with respect to an elasto-plastic deformation law considering isotropic and kinematic hardening and initial plastic orthotropy.

1 Introduction

The successful numerical simulation of the mechanical behaviour of components and structures requires the implementation of suitable material models in Finite Element codes and the sufficient knowledge of the material parameters. As the material parameters are not measurable directly, they have to be identified, solving an inverse problem, which is in general approximated by an optimization problem. That is, the identification of material parameters was formulated as the problem of adjusting the parameters $\boldsymbol{p}$ of the model to minimize an objective function until the calculated values of a mechanical quantity $\hat{\boldsymbol{w}}(\boldsymbol{p})$ (e.g. displacements, stresses) match the measured ones $\tilde{\boldsymbol{w}}$ in the sense of a quadratic norm:

$$\Phi(\boldsymbol{p}) = \frac{1}{2} ||\hat{\boldsymbol{w}}(\boldsymbol{p}) - \tilde{\boldsymbol{w}}||_2^2 \longrightarrow \min_{\boldsymbol{p}} . \quad (1)$$

Due to the physically and mathematically idealized nature of the material models and the incompleteness of measured data, which in addition may be incorrect (disturbances, scattering), the identification of material parameters is an ill-posed problem. Particularly, the non-uniqueness of the solution of the optimization problem (existence of local minima) reduces the reliability of the selected material models. Caused by a lack of experimental information, the ill-posedness of the identification problem is specially distinct for the generally used method of the analysis of homogeneous stress-strain states.

A noticeable improvement of the reliability of the identification of material parameters can be obtained, analyzing inhomogeneous displacement fields using the Finite Element Method (FEM) as suggested by Mahnken & Stein[1], Gelin & Ghouati[2], Bohnsack[3], Meuwissen[4]. On the other hand, Görke & Kreißig[5] investigated the sensitivity of this method with regard to several factors. Particularly, the consequences of choosing non-suitable starting values of the parameters to be determined may be non-unique or unstable optimization results.

Kreißig et al.[6] presented a method to identify material parameters analyzing inhomogeneous displacement fields, using the local integration of the deformation law in several material points with typical mechanical behaviour. This method processes less information than a field solution like FEM, but is a much more effective one with regard to the calculation time. This paper presents results of joining two methods of the analysis of inhomogeneous displacement fields in which the local integration of the deformation law in selected material points provides the starting values of the material parameters to be used for the optimization method including the FEM.

2 Experiments on Bending Specimens

All presented experiments have been carried out at the Department of Experimental Mechanics of Chemnitz University of Technology. Particularly for the reason of getting smooth yield curves the austenitic

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X 6 Cr Ni Ti 18-10 steel alloy was chosen. As the specimens were manufactured from a rolled sheet metal, orthotropic material behaviour with initial plastic anisotropy due to the rolling process can be expected. At first we carried out tensile tests and bending tests on straight specimens as represented in Figure 1.

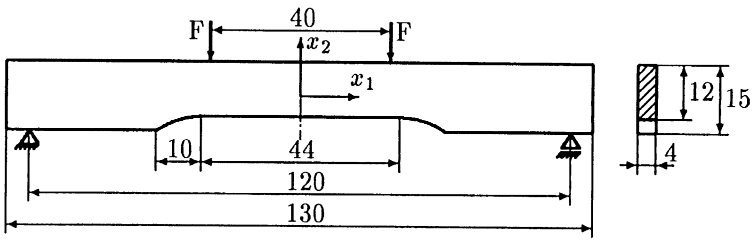

Figure 1: Four-point bending. Geometry of a straight specimen and loading conditions.

The results of experiments have been used for the identification of the elastic parameters, the initial yield locus curve and the uniaxial yield curves for tension and compression.

Figure 2 shows the geometry of a notched bending specimen which has been used to identify the hardening parameters by means of both mentioned methods, analyzing inhomogeneous displacement fields. The displacements have been measured, using the Moiré method. As the measurement points have not necessarily been located on the points needed for the identification (e.g. nodes of the FE-mesh), the displacements were approximated and transformed into the undeformed initial configuration, using an FE-like method (Bohnsack[3]). Simultaneously strains could be calculated at the needed points.

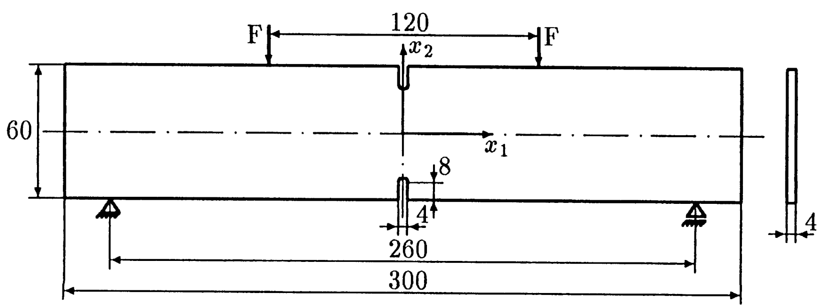

Figure 2: Four-point bending. Geometry of a notched specimen and loading conditions.

3 Optimization and Sensitivity Analysis

As gradientless stochastic or evolutional methods require a large number of solutions of the direct field problem, gradient based methods are preferred for the identification of material parameters, analyzing inhomogeneous displacement fields. It should be remarked that gradient based methods will always follow the direction of a minimum, once it has been found which could be a local but not the global one.

Bohnsack[3] and Görke & Kreißig[5] have achieved the most reliable results of the identification process, using the *Levenberg-Marquardt* gradient based method. Starting from given values $\boldsymbol{p}^0$ of the parameters to be identified, they will be improved by an iterative method:

$$\boldsymbol{p}^{k+1} = \boldsymbol{p}^k + \boldsymbol{s}^k . \tag{2}$$

Within the framework of the *Levenberg-Marquardt* method, the search direction $\boldsymbol{s}^k$ will be determined in the following way:

$$\boldsymbol{s}^k = -\left(\Sigma_{GN}^k + \mu \boldsymbol{I}\right)^{-1} \nabla_{\boldsymbol{p}} \Phi^k \tag{3}$$

with the gradient of the objective function referring to the material parameters $\nabla_{\boldsymbol{p}} \Phi$ and a *Gauß-Newton*-type modification of the matrix of the second partial derivatives Σ_{GN}. As can be seen from eqn (3), the *Levenberg-Marquardt* method corresponds to the method of steepest descent far from the optimal solution with large values of parameter μ. Close to the optimal solution the *Levenberg-Marquardt* method corresponds to the *Gauß-Newton* method with small values of parameter μ which has to be chosen that the search direction is always located in a trust region $\| \boldsymbol{s}^k \| < \delta$ with a given radius δ.

The objective of sensitivity analysis is the determination of the gradient (the first derivatives) of the objective function with respect to the material parameters. Assuming an objective function $\Phi = \Phi(\boldsymbol{p}, \boldsymbol{w}(\boldsymbol{p}))$ depending on a vector of material parameters $\boldsymbol{p}$ and a vector of mechanical quantities $\boldsymbol{w}$, the sensitivity matrix can be determined in the following way:

$$\nabla_{\boldsymbol{p}} \Phi = \frac{d\Phi}{d\boldsymbol{p}} = \frac{\partial \Phi}{\partial \boldsymbol{p}} + \frac{\partial \Phi}{\partial \boldsymbol{w}} \frac{\partial \boldsymbol{w}}{\partial \boldsymbol{p}} . \tag{4}$$

In the present paper the derivatives $\partial\Phi/\partial\boldsymbol{p}$ and $\partial\Phi/\partial\boldsymbol{w}$ are known. Therefore, the estimation of $\nabla_{\boldsymbol{p}} \Phi$ reduces to the determination of the first partial derivatives of the mechanical quantities with respect to the material parameters $\partial w/\partial p$. The vector of mechanical quantities consists of the stresses in the tips of the notches of the specimen shown in Fig. 2 and of the bending momentum and the normal force in the case of the local integration of the deformation law, and it consists of the in-plane displacements using the FEM. As the analytical determination of the derivatives of the mechanical quantities with respect to the material parameters in these cases is not possible, the methods of numerical or semianalytical sensitivity analysis can be used. Semianalytical sensitivity analysis is based on the implicit differentiation of the global equilibrium conditions (not necessary for the local integration of the deformation law) and of the iterated deformation law. This method is more accurate and more effective than numerical sensitivity analysis using finite differences. It was first presented by Mahnken & Stein[1] and Gelin & Ghouati[2]. The application of semianalytical sensitivity analysis on the presented investigations is described in detail by Bohnsack[3].

4 Material Model for Small Anisotropic Elasto-plastic Deformations

The behaviour of elasto-plastic materials with isotropic, kinematic and distorsional hardening regarding small deformations will be characterized by the following relations:

- Relation between the tensors of stress velocity $\dot{\boldsymbol{\sigma}}$ and strain velocity $\dot{\boldsymbol{\varepsilon}}$ with the elasticity matrix $\boldsymbol{C}^{el}$ and the plastic multiplier $\dot{\lambda}$

$$\left(\boldsymbol{C}^{el}\right)^{-1} \cdot\cdot\, \dot{\boldsymbol{\sigma}} + \dot{\lambda}\,\frac{\partial F}{\partial \boldsymbol{\sigma}} - \dot{\boldsymbol{\varepsilon}} = \mathbf{0}. \tag{5}$$

- Evolutional equations for internal variables $\boldsymbol{\kappa}$ (tensorial quantities describing the hardening behaviour)

$$\dot{\boldsymbol{\kappa}} - \dot{\lambda}\,\boldsymbol{q}(\boldsymbol{\sigma}, \boldsymbol{\kappa}, \boldsymbol{p}) = \mathbf{0}. \tag{6}$$

- Yield condition

$$F(\boldsymbol{\sigma}, \boldsymbol{\kappa}, \boldsymbol{p}) = 0. \tag{7}$$

According to the description of the theory of scleronomic plastic flow given in Kreißig[7], a generalized quadratic yield function was assumed in terms of the deviatoric back stresses α_{ij} and the deviatoric stresses $\overset{D}{\sigma}_{ij}$ as the *von Mises* yield function

$$F = \frac{3}{2}\left(\overset{D}{\sigma}_{ij} - \alpha_{ij}\right)\left(\overset{D}{\sigma}_{ij} - \alpha_{ij}\right) - \sigma_F^2 = 0\,. \tag{8}$$

For the presentation of the yield curve as a function of the equivalent plastic strain ε_v^{pl} the modified power law

$$\sigma_F = \sigma_{Fo} + a_1\left[\left(\varepsilon_v^{pl} + a_2\right)^{a_3} - a_2^{a_3}\right] \tag{9}$$

with the yield stress σ_F, and for the evolution of the back stresses *Prager*'s kinematic hardening rule

$$\dot{\alpha}_{ij} = b_1\,\dot{\varepsilon}_{ij}^{pl} \tag{10}$$

have been used.

5 Analysis of Inhomogeneous Displacement Fields

Due to the design of the specimen and the applied loading conditions, on the connecting line between the tips of the notches (furthermore named *ligament*) in the bending specimen shown in Figure 2 a principal stress-strain state can be detected, and immediately in the tips of the notches a uniaxial stress state can be assumed. Regarding the strains as "*external*" loading, the stresses and internal variables can be calculated by the local integration of the deformation law in material points on the ligament without using a global discretization method like the FEM. In the case of the local integration of the deformation law the uniaxial stresses in the tips of the notches, and global quantities as the bending momentum M and the normal force N (which should disappear on the ligament) have been suggested as comparative quantities. The corresponding objective function can be formulated as follows:

$$\Phi(\boldsymbol{p}) = \frac{1}{2}\Bigg[\gamma_1\sum_{i=1}^{n_L}(\hat{\sigma}_M(\boldsymbol{p}) - \tilde{\sigma}_M)^2 + \gamma_2\sum_{i=1}^{n_L}(\hat{\sigma}_N(\boldsymbol{p}) - \tilde{\sigma}_N)^2 \tag{11}$$

$$+\gamma_3\sum_{i=1}^{n_L}(\hat{\sigma}_{11}^{ln}(\boldsymbol{p}) - \tilde{\sigma}_{11}^{ln})^2 + \gamma_4\sum_{i=1}^{n_L}(\hat{\sigma}_{11}^{un}(\boldsymbol{p}) - \tilde{\sigma}_{11}^{un})^2\Bigg]$$

with the number of load steps n_L, weighting factors $\gamma_1 \ldots \gamma_4$ and the stresses in the tip of the upper and the lower notches σ_{11}^{un}, σ_{11}^{ln}. To deal with quantities characterized by similar physical meanings the bending momentum and the normal force have been expressed as affiliated stresses $\sigma_M = 4M/bh^2$ and $\sigma_N = N/bh$. Furthermore, the bending momentum and the normal force have been calculated, using the numerical integration of the stresses on the ligament. Quantities marked by a *hat* represent calculated values, those marked by a *tilde* represent measured values.

As only displacement fields can be measured directly for arbitrary materials and arbitrary load histories, displacements in both $x-$ and $y-$directions can be used as comparative quantities for the identification of material parameters, using the FEM to solve the entire direct field problem. The following corresponding objective function has been formulated in the sense of a least square formulation:

$$\Phi(\boldsymbol{p}) = \frac{1}{2} \sum_{i=1}^{n_L} \sum_{j=1}^{n_T} \left[\left(\{\hat{u}_x(\boldsymbol{p})\}_{ij} - \{\tilde{u}_x\}_{ij} \right)^2 + \left(\{\hat{u}_y(\boldsymbol{p})\}_{ij} - \{\tilde{u}_y\}_{ij} \right)^2 \right] \tag{12}$$

with the number of load steps n_L and the number of material points n_T in which measured and calculated displacements, marked again by *tilde* and *hat* respectively, have been compared.

The combination of both methods for the identification of material parameters for the deformation law described by eqns (8) - (10) analyzing inhomogeneous displacement fields was at first tested on *artificial* measurements, created by an FEM-solution with a given load history consisting of loading, unloading and reloading steps, and given material parameters $\sigma_{Fo} = 220\,\text{MPa}$, $a_1 = 600\,\text{MPa}$, $a_3 = 0.25$ and $b = 750\,\text{MPa}$. As mentioned above, the material parameters identified using gradient-based optimization methods highly depend on their starting values, which may result in the determination of a local minimum different from the global one.

In practice, in investigating new materials it may be difficult to choose a suitable estimation for the starting values of the material parameters. This situation was simulated in the case of artificial measurements.

It turned out that starting from an arbitrary set of material parameters far from the optimal one both of the methods described above found only local minima, which are several due to the different topology of the objective function. The results are summarized in Table 1.

Table 1: Results of the identification of material parameters, analyzing artificial measurements according to eqns (8) - (10) with $a_2 = 10^{-6}$.
Initial orthotropy: α^o_{11} =-16 MPa, α^o_{22} =-6 MPa.

Parameter	Starting values	Optimized values	
		Local integrat.	Field problem
σ_{F_o} in MPa	300.0	241.00	295.58
b in MPa	200.0	504.00	412.89
a_1 in MPa	2000.0	714.00	1841.08
a_3	0.8	0.34	0.66
Approx. calc. time	–	15 min	300 min
Mean deviation of displacem. in mm	0.0215	0.0009	0.00119
σ_{F_o} in MPa	241.00	–	219.92
b in MPa	504.00	–	750.21
a_1 in MPa	714.00	–	599.88
a_3	0.34	–	0.25
Approx. calc. time	–	–	120 min
Mean deviation of displacem. in mm	0.0009	–	$8.74 \cdot 10^{-7}$

Due to the less complex topology of the objective function, which presumably contains less local minima, the solution detected, using the local integration of the deformation law, is a better one with a lower mean deviation of the displacements, but it can hardly not be improved due to its small quantity of information. Using the optimized solution of the method of the local integration of the deformation law as starting values for the analysis of the entire displacement fields by FEM, the global minimum was found (see Table 1). The combination of both methods for the identification of material parameters analyzing inhomogeneous displacement fields improves the result of the optimization process, and is more effective in comparison with using only a field method like FEM.

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The experience taken from the investigations with artificial measurements could be confirmed, analyzing real bending experiments on specimens of the X 6 Cr Ni Ti 18-10 steel alloy, as shown in Table 2.

Table 2: Results of the identification of material parameters, analyzing real measurements for X 6 Cr Ni Ti 18-10 steel alloy according to eqns (8) - (10) with $a_2 = 10^{-6}$, σ_{F_o} =220 Mpa.
Initial orthotropy: α^o_{11} =-8.3 MPa, α^o_{22} =-3.2 MPa.

Parameter	Starting values	Optimized values	
		Local integrat.	Field problem
b in MPa	550.0	1956.00	588.64
a_1 in MPa	440.0	372.00	429.30
a_3	0.1	0.23	0.23
Approx. calc. time	–	5 min	135 min
Mean deviatioan of displacem. in mm	0.0447	0.0185	0.0258
b in MPa	1956.00	–	2793.31
a_1 in MPa	372.00	–	640.53
a_3	0.23	–	0.43
Approx. calc. time	–	–	105 min
Mean deviation of displacem. in mm	0.0185	–	0.0139

6 Conclusions

The identification of material parameters is an ill-posed inverse optimization problem with non-unique and/or unstable solutions. Most of information about the material could be processed identifying material parameters analyzing inhomogeneous displacement fields, using a field method like the Finite Element Method to solve the direct problem at each optimization step. Due to the complex topology of the objective function with a large number of possible local minima, in this case the result of parameter identification highly depends on the optimization conditions, particularly on the starting values of the parameters to be identified.

As could be shown, a suitable method for an acceptable estimation of these starting values is the identification of material parameters analyzing inhomogeneous displacement fields, using the local integration of the deformation law in selected points. This method is a highly effective one, which permits the investigation of additional aspects of the optimization method as using gradientless methods and regularization algorithms.

The combination of two mentioned methods for the identification of material parameters analyzing inhomogeneous displacement fields was successful in the application to artificial and real measurements. Regarding the results of parameter identification using the method of the local integration of deformation laws as starting values, the result and the convergency speed of the method analyzing the entire displacement field by FEM could be noticeably improved.

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