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Identification of elasto-viscoplastic material parameters by indentation testing and combined finite element modelling and numerical optimization

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Using nanoindentation experiments, the material parameters of an elasto-viscoplastic material model with non-linear isotropic and kinematic hardening are determined by minimizing the least-squares difference between experimental data and results from a finite element model of the indentation test. The objective function is minimized by a gradient-based numerical optimization algorithm. The gradient of the objective function with respect to the material parameters is calculated using the direct differentiation method. The parameter coupling occurring in the indentation test is systematically analyzed, and virtual indentation tests are used to assess the reliability of the material parameter identification method. Experimental nanoindentation curves obtained on an aluminium alloy and annealed copper are analyzed. Objective functions consisting of load versus displacement-into-surface curves are used. The efficiency of the use of residual imprint data resulting from nanoindentation testing in the objective function is investigated in order to assess their appropriateness at such small scales.

1. Introduction

Indentation testing is widely used for determining the hardness of materials through Brinell, Vickers or Rockwell hardness tests. Some simple considerations have also been used for relating the hardness to the initial yield stress [1]. The major interest of indentation and nanoindentation testing lies in the fact that due to the small sampling volume size, local material properties, or coating properties, may be investigated. With the development of depth-sensing instrumented indentation and nanoindentation testing, where the full history of applied load versus indenter displacement-into-surface is monitored, methods have been put forward for determining material parameters. First of all, the pioneering work of [2] has presented a method for determining Young's modulus from indentation testing. In the late nineties, methods have been put forward for identifying more material parameters. In the work of [3], an inverse method based on neural networks has been presented for determining the elasto-plastic material parameters of a constitutive law including metal plasticity with both non-linear isotropic and kinematic hardening. Using a similar approach [4] also developed a method for determining Poisson's ratio. Later on, the neural network-based method was extended to elasto-viscoplastic material behaviour [5]. This method, which relies on the construction of dimensionless functions relating indentation curve characteristics to dimensionless variables defined from the material parameters – in this case by the use of neural networks – has also been applied to simpler material constitutive laws, like simple power law hardening laws, either via the construction of analytical dimensionless functions [6–8] or neural networks [9]. Other methods rely on numerical optimization with analytically approximated indentation curves, either the loading segment of the curves [10] or unloading compliances [11].

In a different approach, an objective function, which quantifies the difference between numerically modelled and experimental indentation curves, is minimized. Hamasak et al. [12] used a multipoint response surface analysis for identifying material parameters of an elasto-viscoplastic constitutive law this way. In [13], a method is presented for determining the material parameters of the Norton–Hoff law for metallic materials using the minimization by gradient-based numerical optimization. Bolzon et al. [14] improved the optimization-based parameter identification method by including residual imprint data into the objective function, i.e. using an aggregate objective function in a multi-objective optimization problem. This method has also been used to identify parameters of anisotropic material behaviour [15] and residual stresses [16].

Concerning the optimization-based methods for minimizing an objective function, it is generally advised to use globally

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convergent optimization algorithms whenever possible. They can take the form of evolutionary algorithms, like simulated annealing or genetic algorithms, or deterministic algorithms like the Simplex method. Genetic or evolutionary algorithms are globally convergent and are the only meaningful choice in multi-objective optimization, which comes however at the price of a large number of objective function evaluations. Gradient-based optimization algorithms, like the Levenbergh–Marquardt or Gauss–Newton algorithm, should only be used in case the objective function can be shown to be convex. However, in the case of indentation testing, gradient-based optimization algorithms are preferred despite this drawback, because in general, they involve less function evaluations as gradient-free optimization methods. In fact, because of the highly non-linear nature of indentation testing, involving geometric, material and contact non-linearities, finite element computations of the indentation test are time-consuming. This is also the reason why the required gradients are not computed using time-consuming finite difference schemes, which involve an additional one or two non-linear finite element calculations per optimization variable. Their main advantage, the possibility to easily use them with black-box finite element solvers, is countered by the large computing effort involved. In order to be computationally more efficient, use is made of fast calculation algorithms of the gradients, either through direct differentiation method or through the adjoint state method. These methods have been developed starting with [17,18], and developed to maturity in the framework of material parameter identification by [19–22] or of shape optimization by [23–31]. Sensitivity analysis in the case of contact modelling is well described in [32,33]. In these methods, either the continuum mechanical equations [23–25] or the discretized equations [19,27] are differentiated. The derivatives of state variables and displacements with respect to some parameters, like material parameters, for example, are coupled via linear relationships, which can be motivated by the chain rule in differentiation, and the gradient can be calculated by a linear update scheme. This is in contrast to the finite difference method, where the calculation of gradient information requires the solution of additional non-linear finite element models. This way, gradient calculations involving the direct differentiation or adjoint state method are much faster than finite difference schemes. In addition to that, the fast differentiation methods are more accurate, as they do not depend on a numerical perturbation like the finite difference method. However, it should be noted that finite difference and the fast differentiation methods may produce locally poor results in case of non-differentiable evolution equations, as shown in [34–36].

A different aspect of material parameter identification using inverse methods is parameter correlation. It has for example been shown in [21] that parameter correlation can impede a reliable parameter identification of mixed isotropic and kinematic plastic hardening laws if no reverse plastic flow is induced in uniaxial testing by applying a compressive load after the tensile cycle. The correlation of the material parameters can be assessed through the correlation or cosine matrices [37], which can be determined from the Hessian or approximated Hessian matrix. A strong correlation leads to near-singular matrices in the optimization algorithms, which also has a strong effect on convergence rates and on the accuracy with which the location of the minimum of the objective function can be determined.

In this paper, the constitutive equations typical for metal plasticity are presented in the first section. In the next section, the objective function and the solution procedure for solving the inverse problem of material parameter identification using numerical optimization are presented. The parameter correlation is analyzed and material parameter identification is assessed using synthetic indentation curves, generated by finite element modelling of the nanoindentation test. In the final section, the described inverse method, which has already been used in the framework of depth-sensing microindentation [16,38], is used at a smaller length scale for identifying material parameters of two metallic materials by the use of real experimental nanoindentation data. In addition to the load-versus-displacement indentation curves, the use of experimental residual imprint data for improving the reliability of the method, reported in [14,16], is used in nanoindentation testing, and the suitability of residual imprint data at such a small length scale is investigated.

2. Constitutive formulations

2.1. Elasticity

The material law considered is an elasto-viscoplastic material model with nine material parameters. A detailed description of such constitutive laws, typical of metallic materials, can be found in [39–42], for example. A multiplicative decomposition of the deformation gradient, $\mathbf{F}$, into elastic and plastic parts, $\mathbf{F}_e$ and $\mathbf{F}_p$, respectively, is used.

$$\mathbf{F} = \mathbf{F}_e\mathbf{F}_p. \tag{1}$$

The deformation gradient is calculated from the current configuration ${}^1\mathbf{x}$ and the reference configuration ${}^0\mathbf{X}$ as

$$\mathbf{F} = \frac{\partial^1\mathbf{x}}{\partial^0\mathbf{X}}. \tag{2}$$

The Kirchhoff stress $\mathbf{S}$ is related to the left Cauchy–Green elastic deformation tensor $\mathbf{B}_e$, which is defined through the elastic deformation gradient $\mathbf{F}_e$ as

$$\mathbf{B}_e = \mathbf{F}_e\mathbf{F}_e^T. \tag{3}$$

A neo-Hookean hyperelastic law according to [43] is used. With the elastic material constants μ and λ and the second order identity tensor $\mathbf{I}$, it reads

$$\mathbf{S} = \mu(\mathbf{B}_e - \mathbf{I}) + \frac{\lambda}{2}\ln(\det \mathbf{B}_e). \tag{4}$$

2.2. Plasticity

In the following section, we consider isotropic plasticity with an associative flow rule, including non-linear isotropic and non-linear kinematic hardening. The variation of the yield limit K^y is described through isotropic hardening, with

$$K^y = \sqrt{\tfrac{2}{3}}(\sigma^{y,0} + R[1 - \exp(-\beta s)]), \tag{5}$$

where s is the plastic arc length, $\sigma^{y,0}$ is the initial uniaxial yield stress, and R and β are the non-linear isotropic hardening parameters. The plastic arc length s is a scalar representing the accumulated plastic strain. The evolution of $\boldsymbol{\alpha}$, an internal variable quantifying kinematic hardening, is treated using the Armstrong–Frederick law with the non-linear kinematic hardening parameters H_{kin} and H_{nl}, brought into a form where the kinematic hardening parameter H_{kin} has the meaning of a stress instead of a slope. This feature enables the definition of a better motivated upper bound of H_{kin} in the optimization, i.e. a maximum expected hardening:

$$\dot{\alpha}_{ij} = \sqrt{\tfrac{2}{3}}H_{nl}H_{kin}\dot{\varepsilon}^p_{ij} - \sqrt{\tfrac{3}{2}}H_{nl}\dot{s}\alpha_{ij}. \tag{6}$$

In that case, the maximum yield stress can be approximated by

$$\sigma_\infty \approx \sigma^{y,0} + R + \tfrac{3}{2}H_{kin}. \tag{7}$$