INDENTATION TESTING PARAMETER IDENTIFICATION USING AN OPTIMIZATION PROCEDURE BASED ON GENETIC ALGORITHMS

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Nanoindentation testing can be used as experimental technique for determining the material parameters. This paper presents a sequential optimization method for determining mechanical material parameters from indentation experiments with inhomogeneous stress and strain fields. The purpose of this inverse problem is to determine the elasto-viscoplastic material parameters that lead to the most accurate agreement between experimental data and indentation simulation results. A sequential combination of an optimization method based on evolutionary genetic algorithms, with a more classical gradient-based optimization algorithm, is proposed. The sequential optimization procedure works as follows: the genetic algorithm is generating starting points, and for each starting point the gradient-based nonlinear optimization solver is launched. The identifiability of material parameters and the reliability of the proposed method are proved by the examples tested so far.

Key words: Indentation testing; Nanoindentation; Parameter identification; Inverse problem; Genetic algorithm; Numerical optimization.

1. INTRODUCTION

The identification of material constitutive parameters based on experimental data is a major issue in solid mechanics, since these parameters are involved in the constitutive models. Indentation/nanoindentation is one of the testing techniques currently available, being used especially in surface engineering, for example in order to characterize the mechanical properties of thin films coated materials. Through refinements and developments in sensor and actuator technology, it has been possible to go from macroscopic indentation testing towards depth-sensing micro- and nanoindentation, thus enabling a local investigation of material behaviour. In practice, nanoindentation is load-driven, the output recorded is the displacement-into-surface.

Commercial nanoindenters software usually provide Young's modulus and hardness. Whereas hardness is a very useful parameter for quantitative evaluation of materials, it does not directly provide true material parameters, like elastic, viscous and plastic parameters. Starting with the pioneering work of [1], it has become possible to evaluate true material parameters (like the Young's modulus) from indentation testing, and subsequently, methods have been put forward for estimating the yield strength. In simple experiments with uniaxial stress fields, some material parameters can be directly read from experimental curves at characteristic points (like maximum values, slopes) or at the onset of non-linear behaviour. As for the material parameters that cannot be determined in such direct manner, e.g., plasticity parameters for metals, more elaborate methods involving numerical modeling of the indentation test have been proposed.

The purpose of the parameter identification is to determine the elasto-viscoplastic parameters that lead to the most accurate agreement between experimental data and nanoindentation simulation results. This is an inverse problem, because the material parameters cannot be calculated directly by solving a boundary value problem. An objective function is defined in order to quantify the difference between experimental input curves and modeled nanoindentation output, to be minimized by means of an optimization procedure. Several approaches can be used, from classical numerical optimization to neural networks.

The classical numerical optimization consists in performing a non-linear regression using a variety of methods. Basic methods like genetic algorithms, simplex method etc, use objective function values only, whereas more advanced gradient-based numerical optimization methods, like Gauss-Newton or Levenberg-Marquardt, use the objective function derivative and even the second order derivative, the so-called Hessian matrix [10]. Whereas for analytical solutions derivatives can easily be calculated, in the case of numerical solution methods, which are very often incremental solution schemes, the calculation of the derivatives, also called sensitivity analysis, is less straight-forward.

Neural networks represent a second interesting approach for solving the parameter identification inverse problem. For example, neural network-based procedures have been developed for determining the Poisson ratio [15], or non-linear kinematic and isotropic hardening parameters [13]. A similar approach has been developed, for a simpler constitutive law for plasticity with power law hardening, by using response surfaces whose coefficients have been determined through a large number of numerical experiments [12].

This paper continues the work started in [10], where only elasto-plastic material indentation was considered and where only classical gradient-based optimization algorithms were used. The current paper presents a sequential optimization method for determining elasto-viscoplastic material parameters from nanoindentation experiments. More precisely, a sequential combination of an optimization method based on evolutionary genetic algorithms [21-24], with a more classical gradient-based optimization algorithm, is proposed: the genetic algorithm is generating starting points, and for each starting point a gradient-based optimization is performed by Gauss-Newton iterations with approximated Hessian matrix and fixed bounds. KNITRO [25] is used as gradient-based optimization solver. The identifiability of material parameters and the reliability of the proposed method are proved by the examples tested so far.

2. ELASTO-VISCOPLASTIC MATERIAL BEHAVIOUR

In what concerns the plasticity behaviour, associative plasticity with isotropic J2-flow theory is considered. Plastic yielding is governed by the yield function f, defined as follows:

$$f = \left\| \left(\mathbf{S} - \boldsymbol{\alpha} \right) \right\| - K^{y} \qquad \begin{cases} f < 0, \text{ elastic} \\ f \ge 0, \text{ viscoplastic} \end{cases}$$
(1)

where K^y is the yield limit, α the back-stress, an internal deviatoric variable, and **S** the stress deviator, calculated from the Cauchy stress σ . Viscoplasticity is included into the constitutive model by including a viscosity-dependent term into the consistency condition, for $f \ge 0$ [20]:

$$f = \left\| \left(\mathbf{S} - \boldsymbol{a} \right) \right\| - K^{y} - \sqrt{\frac{2}{3}} \left(\eta \dot{s} \right)^{\frac{1}{m}} = 0.$$
⁽²⁾

In fact, viscosity plays and important role in indentation testing [11]. Since the beginning of the unloading phase yields the information needed for determining the Young's modulus, viscosity-induced rounding of the indentation curves during unloading has a significant impact on the material parameter identification. Generally speaking, viscosity in metallic materials only plays a role at higher temperatures. However, viscosity also takes place at room temperature because of high stresses occurring below the indenter tip. Attempts have been made to include viscous material behaviour into the material parameter identification procedures using indentation testing [4,16]. However, a strong correlation between some material parameters was found, prohibiting a stable and unique material parameter identification [4].

The yield limit K^{y} evolves according to the isotropic hardening law of Voce, without linear term:

$$K^{y} = \sqrt{\frac{2}{3}} \left[Y^{0} + R \left(1 - \exp(-\beta s) \right) \right],$$
(3)

where *s* is the plastic arc length, i.e. the accumulated plastic strain magnitude, Y^0 is the initial uniaxial yield stress, and *R* and β are the non-linear isotropic hardening parameters. Using the rates of the plastic strain ε_p and arc length *s*, kinematic hardening is modeled using the Armstrong-Frederick law with the non-linear kinematic hardening parameters H_{kin} and H_{nl} :

$$\dot{\boldsymbol{\alpha}} = \boldsymbol{H}_{\rm nl} \left(\boldsymbol{H}_{\rm kin} \dot{\boldsymbol{\varepsilon}}_{\rm p} - \sqrt{\frac{3}{2}} \dot{\boldsymbol{s}} \boldsymbol{\alpha} \right). \tag{4}$$

This non-standard form of the Armstrong-Frederick law is used in order to give H_{kin} the meaning of a stress, which can be better traced on the stress-strain curve at plastic saturation.

The hypo-elastic material behaviour is described using Hooke's law, which relates the Cauchy stress σ to the elastic strains ϵ_{el} , using the fourth-order elasticity tensor C :

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}_{\mathrm{el}} \,. \tag{5}$$

Based on the constitutive equations (1)-(5), the stress update equations are formulated, incrementally, in order to simulate the evolution of the indentation process. Details of the incremental formulation of the stress update equations, written in a rotation-neutralized frame, can be found in [9-10,17].

The second major issue concerning the material behaviour is the sensitivity analysis, i.e. the calculation of the derivatives of the state variables with respect to the material parameters. The easiest approach for calculating derivatives is to use a finite difference scheme. However, this method is very time-consuming and prone to numerical error. Two other methods exist for calculating the exact derivatives for inelastic material models with reduced computing effort: the adjoint state method [3-4] and the direct differentiation method [5-7]. The direct differentiation method is used in this paper, see [9] for details. In both methods, the derivatives are calculated by a linear update scheme, as opposed to the non-linear calculations used in finite difference schemes, which lead to a large reduction in computational effort. Contact sensitivity analysis has been treated intensively by [8].

3. FINITE ELEMENT MODEL OF THE INDENTATION TEST

The uniaxial indentation test consists in pushing a hard indenter vertically into the plane surface of the material. The nanoindenter records the load P and the penetration h of the indenter tip into the surface, where the penetration h is the total displacement of the specimen contact surface at the vertical line of symmetry.



Fig. 1. Axisymmetric finite element model of the indentation test using a conical indenter with a spherical tip radius of 5 µm

Fig.1 shows the finite element model of the indentation test, i.e., an axisymmetric model discretizing both the indenter and the specimen as flexible bodies. The spherical indenter has a tip radius of 5 μ m and the overall shape is a cone with an opening angle of 60°. The material behaviour of the indenter is hypo-elastic, with a Young's modulus of 1004 GPa and a Poisson's ratio of 0.07. Nine-noded, fully integrated quadratic elements with displacement degrees of freedom have been used because their convergence behaviour is very good. However, such finite elements require larger computing times. The specimen consists of 100 elements and the indenter consists of 54 elements, as shown in Fig.1. Contact constraints are fulfilled by using C²continuous quadratic node-to-segment contact elements with a modified C²-continuous logarithmic barrier potential according to [18]. A simple penalty algorithm with intermediate loops [19] has been used, where the barrier parameter p of the modified contact potential is increased between the intermediate loops from p^{\min} at the beginning of the increment until p^{\max} is reached after M^{\max} intermediate loops. At the end of each intermediate loop, an extrapolation according to [19] is performed for convergence improving. A line search method is included into the Newton-Raphson iteration loop in order to improve overall convergence. The finite element calculations are performed under load control. The size of the specimen region was chosen in such a way that it is equivalent to a semi-infinite body, i.e. more than ten times the processing zone.

4. OPTIMIZATION PROCEDURE FOR PARAMETER IDENTIFICATION

The purpose is to determine the elasto-viscoplastic material parameters that lead to the most accurate agreement between experimental data and simulation results. In this paper, synthetic experimental curves are used as input curves in the parameter identification method. These synthetic experimental curves are calculated by finite element modeling and therefore considering known material parameters.

For the indentation test, the objective function to be minimized by a numerical optimization algorithm is made up of the difference or gap between the experimental and modeled displacement-into-surface, \overline{h} and h, respectively, which are a function of the independent load *P*:

$$\Xi = \frac{1}{2} \sum_{k=1}^{N} \left[h \left(P^k \right) - \overline{h} \left(P^k \right) \right]^2.$$
(6)

In the case of plasticity, a residual imprint is created during the indentation test, and its geometry, generally its cross-sectional profile, may also be included into the objective function [2], provided it can be determined experimentally by either atomic-force-microscopy or white-light-interferometry, in general after total load removal. However, in the present study, the system response considered is only the displacement-into-surface, without considering also the residual imprint.

A gradient-based optimization algorithm requires the derivatives
$$\frac{\partial \Xi}{\partial \kappa_i}$$
 of the objective function with

respect to the material parameters κ_i . It should be noted that the derivatives of the objective function with respect to the different material parameters differ by several orders of magnitude, and this fact adversely affects the convergence of the numerical optimization algorithms. Thus, the material parameters must be scaled by the gradient of the initial solution, normalized by its largest magnitude. The Hessian matrix is:

$$H_{ij} = \frac{\partial^2 \Xi}{\partial \kappa_i \partial \kappa_j} = \sum_{k=1}^{N} \left[\frac{\partial h(P^k)}{\partial \kappa_i} \frac{\partial h(P^k)}{\partial \kappa_j} - \left[h(P^k) - \overline{h}(P^k) \right] \frac{\partial h^2(P^k)}{\partial \kappa_i \partial \kappa_j} \right] \cong \sum_{k=1}^{N} \frac{\partial h(P^k)}{\partial \kappa_i} \frac{\partial h(P^k)}{\partial \kappa_j}.$$
 (7)

The second term in (7) can be neglected, because in the case of multiple material parameters, the computing times will increase significantly. In case of numerical noise, the use of such second order derivatives becomes highly questionable, especially if the initial solution is far from the final solution.

A gradient-based minimization algorithm, such as the Gauss-Newton algorithm used by KNITRO nonlinear optimization solver [25], iteratively calculates the material parameters using:

$$\mathbf{\kappa}^{n+1} = \mathbf{\kappa}^n - \mu^n \left(\mathbf{H}^n\right)^{-1} \frac{\partial \Xi}{\partial \mathbf{\kappa}^n},\tag{8}$$

where *n* denotes here the iteration number, κ is the vector of material parameters κ_i to be identified, and μ^n is the parameter of the line search algorithm performed inside the Gauss-Newton method to find the lowest value of the objective function Ξ along the search direction. The approximated Hessian matrix \mathbf{H}^n given by (7) has to be positive definite in order to provide that the search direction is a descent, convergent direction.

The sequential optimization procedure proposed in this paper is based on a genetic algorithm driver and on the numerical optimization solver. The purpose is to identify the following nine parameters corresponding to an elasto-viscoplastic material behaviour: the elasticity parameters, i.e. Young's modulus E and Poisson's ratio v, the viscosity η and the viscosity exponent *m*, and finally the plasticity parameters: the initial uniaxial yield stress Y^0 , the non-linear isotropic hardening parameters *R* and β and the non-linear kinematic hardening parameters H_{kin} and H_{nl} . The goal is to adjust these nine parameters, starting from an initial guess or estimation, in order to minimize the objective function Ξ defined by (6).

Among the evolutionary algorithms, the genetic algorithms (GA) represent one of the most popular methods for objective function minimization. In this work, the Fortran Genetic Algorithm driver proposed by [21] was used. The GA code initializes a random sample of chromosomes with the nine parameters to be optimized using the GA approach, i.e. evolution via survival of the fittest (the chromosome corresponding to the smallest objective function). The selection scheme used is tournament selection with a shuffling technique for choosing random pairs for mating [21]. The main GA parameters, such as the population size, number of maximum generations, crossover probability (=0.5), jump mutation probability (=0.03) and creep mutation probability (=0.2) have been adapted to the specificity of our inverse problem. Each parameter to identify was coded on 6 bits, so the permitted interval between the lower and the upper bounds for each parameter was divided into 2^6 =64 equal subintervals, leading to a total chromosome length of $9\times6=54$ bits.

Running the GA on its own is not a very efficient technique, due to a long computational time. Also, one can pass quite close to the solution, without finding it very precisely. On the other hand, performing just simple runs of a classical gradient-based optimization algorithm, such as Gauss-Newton or Levenberg-Marquardt, can lead to local minima. In fact, for a gradient-based optimization algorithm to converge, it is necessary to start the descent towards the solution from an appropriate initial guess, so that to place the optimization problem closer to its global minimum [25]. Otherwise, even a powerful nonlinear optimization solver can misleadingly converge towards a local minimum, while the global minimum is located elsewhere.

To overcome the disadvantages of GA or gradient-based optimization algorithms working separately, this paper proposes a sequential optimization procedure where the GA driver is used to generate starting points for launching the numerical optimization solver. The proposed GA+OPT sequential optimization procedure works as follows: the GA is generating starting points, and for each starting point the gradient-based optimization is launched, performing Gauss-Newton iterations with approximated Hessian matrix and fixed bounds (see (8)). The number of Gauss-Newton iterations per each numerical optimization launch is restricted to only 10 iterations. But, since GA will always retain the best chromosomes, the convergence towards the solution will continue during next GA generations. So, if one has 10 generations and only 10 Gauss-Newton iterations for each gradient-based optimization launch, then for some best chromosome this divided-by-generations job will be equivalent with performing $10 \times 10 = 100$ overall Gauss-Newton iterations.

5. NUMERICAL VALIDATION OF THE OPTIMIZATION PROCEDURE

In order to assess its efficiency and its robustness, the GA+OPT sequential optimization procedure was tested on five parameter identification cases, numbered Test-1 until Test-5. Table 1 presents the values of the material parameters to be identified for these five tests. Test-1 concerns a single load cycle (load-hold-unload), while Test-2 until Test-5 concern double load cycles (load-hold-unload-reload-hold-unload).

Test N°	E [MPa]	ν[-]	Y^0 [MPa]	R [MPa]	β[-]	H _{kin} [MPa]	<i>H</i> _{nl} [-]	$\eta [(MPa)^m s]$	<i>m</i> [-]
Test-1	183199.62	0.1530	610.30	663.27	40.93	623.42	31.23	4704.92	8.59
Test-2	491032.00	0.4100	112.00	550.00	11.00	230.00	5.50	400.00	4.50
Test-3	133833.70	0.2108	317.13	104.33	6.52	165.54	10.59	2352.84	2.56
Test-4	262101.40	0.2840	965.66	405.71	13.70	348.21	7.42	1256.10	3.18
Test-5	366945.24	0.4256	887.10	720.02	4.11	820.06	5.52	1224.67	6.62

Table 1. Material parameters to be identified in Test-1, Test-2, Test-3, Test-4 and Test-5

Table 2 presents the lower and the upper bounds allowed for these material parameters, since one deals with a fixed bounds optimization.

BOUNDS	E [MPa]	v [-]	Y^0 [MPa]	R [MPa]	β[-]	H _{kin} [MPa]	$H_{\rm nl}$ [-]	$\eta [(MPa)^m s]$	<i>m</i> [-]
Lower	1000	0.10	1	1	1	1	1	1	1
Upper	1000000	0.49	10000	5000	50	5000	50	20000	10

Table 2. Lower and upper bounds of the nine material parameters to be identified

The parameter identifications have been performed using so-called virtual experimental curves, generated by the same finite element model used to simulate the direct problem, in order to avoid systematic errors in the experimental data. The true material parameters corresponding to such virtual experimental curves are obviously known exactly. Figure 2 shows the load versus displacement-into-surface virtual experimental curve corresponding to the materials considered in Test-1 until Test-5.



Fig. 2. Load versus displacement-into-surface virtual experimental curve corresponding to the parameters of the materials considered in Test-1, Test-2, Test-3, Test-4 and respectively Test-5

The material parameter identification procedure is started with different sets of material parameters, called starting points. In the GA, each chromosome has a different starting point. Starting from these initial guess points, the optimization procedure should ideally converge to the true material parameters.

Fig.3 shows the evolutions of the logarithm $log(\Xi)$ of the objective function Ξ , when applying two different methods: the method using only GA (with a population size of 50 and running 100 generations), respectively the proposed GA+OPT sequential optimization procedure (with GA driver characterized by a population size of 7 and running 10 such generations, and with 10 the maximum number of Gauss-Newton iterations performed during one optimization launch by the GA driver). Table 3 shows, for the method using only GA, the relative errors in the identified material parameters with respect to the true values.

Test N°	Ε	ν	Y^0	R	β	$H_{ m kin}$	$H_{\rm nl}$	η	т
Test-1	2.7%	23.3%	8.2%	42.3%	79.9%	12.5%	9.1%	23.5%	7.0%
Test-2	1.7%	8.8%	2.1%	6.2%	36.0%	4.6%	42.3%	37.7%	7.9%
Test-3	2.8%	12.5%	12.5%	14.9%	13.9%	18.0%	52.1%	60.8%	18.1%
Test-4	2.1%	21.7%	1.5%	1.4%	7.4%	1.7%	2.1%	43.7%	44.4%
Test-5	6.5%	1.8%	0.9%	12.6%	7.8%	4.2%	9.0%	6.6%	7.6%

Table 3. Relative errors in the identified material parameters, for all five tests, when using the GA-only method

Finally, Table 4 shows the relative errors in the identified material parameters, for all five tests, when using the GA+OPT sequential optimization procedure. From Table 3, it can be concluded that running only the GA, without numerical optimization, is not a very efficient technique. Big relative errors are obtained, thus one cannot speak of reliable parameter identification using the GA-only method. In what concerns the computing time, one objective function calculation takes around 2 minutes, so a generation of this GA-only method with a population size of 50 chromosomes takes $50 \times 2=100$ minutes, so for 100 generations one needs $100 \times 100=10000$ min $\cong 167$ h $\cong 7$ days, all this on a 2.19 GHz AMD Turion 64 Mobile processor.

Test N°	Ε	ν	Y^0	R	β	$H_{\rm kin}$	$H_{\rm nl}$	η	т
Test-1	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	1.3%	0.3%
Test-2	0.1%	0.1%	0.0%	0.1%	0.0%	0.0%	0.1%	2.4%	9.0%
Test-3	0.0%	0.2%	0.0%	0.0%	0.1%	0.0%	0.1%	4.4%	1.2%
Test-4	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	1.0%	0.9%
Test-5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.1%	0.1%

Table 4. Relative errors in the identified material parameters, when using the GA+OPT sequential optimization procedure



Fig. 3. Evolutions of the logarithm $log(\Xi)$ of the objective function Ξ , for all five tests, performed by two methods: GA-only (left graph), versus GA+OPT (right graph)

In what concerns the proposed GA+OPT sequential optimization procedure, it worked perfectly for all five tests (see Table 4). Only for the viscosity parameters there are still some small relative errors in the identified parameters, but not bigger than 10%. This error level for the viscosity parameters was found to be in good agreement with the results reported in [4,16], and is probably related to the strong correlation between the viscous parameters, in addition to the small overstresses involved at room temperature. As for the elasticity and plasticity parameters, the error is never bigger than 1%, so the proposed GA+OPT method is very reliable. As for the computing time, an optimization launch performing 10 Gauss-Newton iterations, with an average of five function evaluations due to the line-search method, takes around 60 minutes, so a generation of this GA+OPT method with a population size of 7 chromosomes needs around 420 minutes, so for 10 such GA+OPT generations one needs about $10 \times 420 = 4200 \text{ min} \cong 70 \text{ h} \cong 2.9$ days of computing time.

6. CONCLUSIONS

The goal of the parameter identification inverse problem is to determine the unknown elastoviscoplastic material parameters of a specimen by reproducing the measured experimental indentation data on that specimen by finite element modeling. This inverse problem is solved by the proposed hybrid genetic and gradient-based sequential optimization method, GA+OPT, working as follows: the GA is generating several starting points, and for each starting point the gradient-based nonlinear optimization solver is launched. This sequential procedure increases significantly the likelihood of finding the true global minimum, by combining the advantages of both GA combinatorial technique and a powerful numerical optimization solver. The tests performed so far proved that the GA+OPT method performs reliable and efficient parameter identifications associated with inelastic isotropic material indentation testing. Further investigations will include additional data from residual imprint mapping and will consider more complex changes in the load cycles of the indentation test. Experimental noise needs to be taken into account as well, in order to better approach real indentation testing.

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