

PARAMETERS IDENTIFICATION OF MATERIAL MODELS BASED ON THE INVERSE ANALYSIS

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The paper presents an application of the inverse analysis to the identification of two models: a phase transformation model and a rheological model. The optimization algorithm for the inverse analysis was tested for various techniques of searching for the minimum: derivative-free and gradient methods, as well as genetic algorithms. Simulation results were validated for microalloyed niobium steel. An optimization strategy, which is adequate for the inverse analysis, is suggested.

Keywords: inverse analysis, phase transformation, internal variable model

1. Introduction

Numerical modelling of various technological processes, including metal forming, is a commonly used method in research and technological design. The simulation of various phenomena involved in thermomechanical steel processing requires knowledge regarding numerous parameters which characterize this process, including a material model and boundary conditions. The character of such models is generally known, but the determination of coefficients in the models for particular materials usually presents problems. In the case of metal forming, the stress strain characteristic, called the flow stress, is crucial to the simulation process. This characteristic is determined based on plastometric tests, which are performed in conditions close to those appearing in the industrial practice. Due to inhomogeneities of deformation and temperature in these tests, their interpretation is difficult and often erroneous. In a number of papers, see, e.g. (Boyer and Massoni, 1999; Szeliga and Pietrzyk, 2002), it is shown that coupling the model of the test with optimization techniques leads to an efficient tool, which allows for an analysis of the plastometric tests. This tool may account for the common disturbances which appear in the tests. Although this approach has numerous advantages, long computation time is its main disadvantage. The computational cost of the inverse analysis depends mainly on the applied optimization algorithms. Gradient and derivative-free techniques have been used in a majority of the published works (Boyer and Massoni 2001; Forestier *et al.*, 2002; Szyndler *et al.*, 2001a; 2001b), but several examples of applying evolutionary algorithms can also be found (Braasch and Estrin, 1993; Gawąd and Szeliga, 2002; Ta-

lar *et al.*, 2002), in particular for a primary search and for constraining the search domain. It should be emphasized, however, that each optimization task requires an individual approach regarding the selection of optimization techniques. This selection depends on the form of the material model that is identified, and on the number of the optimization variables.

The present paper is aimed at developing an optimization strategy for the inverse analysis. The objective is to search for a method that would allow for a sufficiently accurate determination of the minimum regardless of the material model which is identified, and of the starting point within certain limits. The developed optimization algorithm was validated for microalloyed niobium steel deformed in a two-phase region of temperatures.

2. Inverse Analysis

The determination of coefficients in models of deformed materials on the basis of the results of plastometric tests constitutes the objective of the inverse analysis (Lenard *et al.*, 1999; Szeliga and Pietrzyk, 2002). The algorithm, which is used in the present work, is composed of the following three parts:

- Experiments, which supply the measured output parameters used as the input for optimization procedures.
- Solution of a direct problem, which is based on a finite-element model used for the simulation of a selected plastometric test or a dilatometric test.
- Optimization procedures, which allow for the identification of coefficients in the models.

The module of the direct problem determines output test parameters, which are grouped in the vector \mathbf{d} , as a function of the process parameters grouped in the vector \mathbf{p} and coefficients of the material model grouped in the vector \mathbf{x} :

$$\mathbf{d} = F(\mathbf{x}, \mathbf{p}). \quad (1)$$

The vector \mathbf{x} is unknown in the inverse analysis, while the remaining two vectors, \mathbf{d} and \mathbf{p} , are given. The components of the vector \mathbf{d} are calculated by the direct problem model (\mathbf{d}^c), and measured in the tests (\mathbf{d}^m). The identification of \mathbf{x} is performed by searching for a minimum of the cost function, which is usually defined as the root mean square error (error in the Euclidean norm) between the calculated (\mathbf{d}^c) and measured (\mathbf{d}^m) output parameters:

$$\Phi(\mathbf{x}) = \sum_{i=1}^n \beta_i [\mathbf{d}_i^c(\mathbf{x}) - \mathbf{d}_i^m]^2, \quad (2)$$

where β_i are weights.

2.1. Direct Problem

Two tests are investigated here, namely, the axisymmetrical compression test and the dilatometric test. Models of these tests are the direct problem models. The former test is simulated using the finite-element approach. The solution based on the so-called flow formulation coupled with the solution of the heat transfer partial differential equation is described in detail in (Lenard et al., 1999). In the mechanical part of the model the fields of velocities, strains and stresses are calculated from the condition for the minimum of the following functional:

$$J = \int_V \sigma_i \dot{\epsilon} dV + \lambda \int_V \dot{\epsilon}_V dV + \int_S F v_s dS, \quad (3)$$

where V is the control volume, S is the contact surface, σ_i is the effective stress (according to the Huber-Mises yield criterion, it is equal to the flow stress σ_p), $\dot{\epsilon}$ is the effective strain rate, λ is the Lagrange multiplier, v_s is the slip velocity, and F is the contact force. The discretization of (3) gives

$$J = \int_V \sigma_p \sqrt{\mathbf{B}^T \mathbf{v}^T \mathbf{v} \mathbf{B}} dV + \lambda \int_V \mathbf{c}^T \mathbf{B} \mathbf{v} dV - \int_S \mathbf{f}^T \mathbf{v} dS, \quad (4)$$

where \mathbf{B} is the matrix of the derivatives of shape functions, \mathbf{v} is the vector of nodal velocities, \mathbf{f} is the vector of boundary tractions, and \mathbf{c} is a vector which imposes the incompressibility condition.

The differentiation of (4) with respect to \mathbf{v}^T and to λ yields a set of non-linear equations, which is linearized using the Newton-Raphson technique:

$$\begin{bmatrix} \frac{\partial^2 J}{\partial \mathbf{v} \partial \mathbf{v}^T} & \left\{ \frac{\partial^2 J}{\partial \mathbf{v} \partial \lambda} \right\}^T \\ \frac{\partial^2 J}{\partial \mathbf{v} \partial \lambda} & 0 \end{bmatrix} \begin{Bmatrix} \Delta \mathbf{v} \\ \lambda \end{Bmatrix} = \begin{Bmatrix} \frac{\partial J}{\partial \mathbf{v}^T} \\ \frac{\partial J}{\partial \lambda} \end{Bmatrix}. \quad (5)$$

An iterative solution of the set of linear equations yields a real velocity field. In the flow theory of plasticity, strain rates ($\dot{\boldsymbol{\epsilon}}$) are related to stresses ($\boldsymbol{\sigma}$) by the Levy-Mises flow rule

$$\boldsymbol{\sigma} = \frac{2\sigma_p}{3\dot{\epsilon}_i} \dot{\boldsymbol{\epsilon}}, \quad (6)$$

where $\boldsymbol{\sigma}$ and $\dot{\boldsymbol{\epsilon}}$ are the vectors containing components of the stress and strain rate tensors, respectively.

The traction boundary condition at the free surface is either a zero traction or, ordinarily, at most uniform hydrostatic pressure. However, the boundary conditions along the die-workpiece interface S are mixed. In general, neither the velocity nor the force can be prescribed completely along this interface. This is due to the fact that the direction of the relative velocity is not known *a priori*. In order to deal with this problem, a velocity-dependent frictional stress is used (Kobayashi et al., 1989):

$$\mathbf{f} = \frac{2m\sigma_p}{\pi} \arctan\left(\frac{|v_s|}{v_0}\right) \mathbf{d}, \quad (7)$$

where v_s is the slip velocity, v_0 is a positive number, which is small compared to v_s , and \mathbf{d} is the unit vector in the direction opposite to the relative sliding.

The flow formulation is coupled with the finite-element solution of the Fourier heat transfer equation:

$$\nabla k(T) \nabla T + Q(T) = c_p(T) \rho(T) \frac{\partial T}{\partial t}, \quad (8)$$

where $k(T)$ is conductivity, $Q(T)$ is the heat generation rate due to deformation work, $c_p(T)$ is specific heat, $\rho(T)$ is density, T is temperature and t is time.

The following boundary conditions are used in the solution:

$$k \frac{\partial T}{\partial \mathbf{n}} = q + \alpha (T_a - T), \quad (9)$$

where α is the heat transfer coefficient, T_a is the surrounding temperature or the tool temperature, q is the heat flux due to friction, and \mathbf{n} is the unit vector normal to the surface.

The heat transfer coefficient was selected as 10000 W/m² K on the basis of data presented in (Pietrzyk et al., 1994). The Galerkin integration scheme is applied for a non-stationary solution. More details regarding both a mechanical and a thermal model can be found in (Lenard

et al., 1999). Descriptions of numerous successful applications of this model combined with the inverse analysis for single phase materials are presented in (Szeliga and Pietrzyk, 2002; Szyndler *et al.*, 2001a; 2001b).

The relation describing the flow stress σ_p in (6) for materials deformed in the two-phase region of temperatures consists of two parts. The first part contains a set of equations describing the flow stress separately for each single phase. The second part is the phase transformation model. Both parts are combined by the rule of mixture (Bodin *et al.*, 2001). The following equation was selected for the description of the flow stress σ_p for the phases of ferrite (Gavrus *et al.*, 1996):

$$\sigma_p = \sqrt{3} \left[WK_0 \varepsilon^n \exp\left(\frac{\beta}{T}\right) + (1 - W)K_{\text{sat}} \exp\left(\frac{\beta_{\text{sat}}}{T}\right) \right] (\sqrt{3}\dot{\varepsilon})^m, \quad (10)$$

$$W = \exp(-R_0\varepsilon),$$

where m , n , R_0 , K_0 , K_{sat} , β_{sat} , β are coefficients, ε is the strain, $\dot{\varepsilon}$ is the strain rate, and T is the temperature [K].

The flow stress model for austenite has to account for dynamic phenomena in the material. Therefore, the internal variable model was selected. The details of this model are given in (Szyndler *et al.*, 2001b) and only main equations are briefly reported here. The flow stress in this model is calculated as

$$\sigma_p = \sigma_0 + \alpha b \mu \sqrt{\rho}, \quad (11)$$

where α is a coefficient, b is Burger's vector, μ is the shear modulus and σ_0 is the stress accounting for elastic deformation.

The evolution of dislocation populations takes into account the restoration processes and is given by

$$\frac{d\rho(t)}{dt} = \frac{\dot{\varepsilon}}{bl} - k_2\rho(t) - \frac{A_3\mu b^2}{6D_\gamma}\rho(t)R(\rho(t) - \rho_{cr}), \quad (12)$$

where ρ_{cr} is the critical dislocation density calculated as a function of the Zener-Hollomon parameter, D_γ is the austenite grain size, t is time, and l is the average free path of dislocations,

$$l = A_0 Z^{-A_1}. \quad (13)$$

The function R in (12) is calculated as

$$R(\rho(\tau) - \rho_{cr}) = \begin{cases} 0 & \text{if } \rho < \rho_{cr}, \\ \rho(t - t_{cr}) & \text{if } \rho \geq \rho_{cr}, \end{cases} \quad (14)$$

where t_{cr} is the time at the beginning of dynamic recrystallization.

The coefficients k_2 and A_3 are temperature dependent, according to the Arrhenius law:

$$k_2 = k_{20} \exp\left(\frac{10^3 Q_s}{RT}\right), \quad (15)$$

$$A_3 = A_{30} \exp\left(\frac{10^3 Q_m}{RT}\right), \quad (16)$$

where Q_m is the activation energy for grain boundary mobility, Q_s is the activation energy for self-diffusion, and R is the gas constant.

Phase transformation models are composed of equations describing incubation time and the kinetics of ferritic, pearlitic and bainitic transformations. Only the ferritic transformation is considered in the present work. The transformation starts at an equilibrium temperature A_{e3} and its evolution is determined in accordance with

$$\tau_f = \frac{a_1}{(A_{e3} - T)^{a_3}} \exp\left(\frac{1000a_2}{RT}\right), \quad (17)$$

$$\frac{df_f}{dt} = a_4 (SIG^3)^{0.25} \left[\ln\left(\frac{1}{1 - f_f}\right) \right]^{0.75} (1 - f_f), \quad (18)$$

$$\frac{df_f}{dt} = a_5 \frac{6}{D_\gamma} G (1 - f_f), \quad (19)$$

where f_f is the volume fraction of the ferrite, τ_f is the incubation time for the ferritic transformation, G is the rate of the transformation, S is a specific area of the grain boundary, D_γ is the austenite grain size, and I is the rate of nucleation:

$$I = T^{-0.5} D \exp\left(\frac{a_6}{RT_K \Delta G}\right), \quad (20)$$

where D is the diffusion coefficient and ΔG is the free Gibbs energy.

Equation (18) describes the progress of the transformation when the mechanisms of nucleation and growth are active. Equation (19) is responsible for site saturation. The remaining equations used to calculate the parameters in the relationship (18), as well as a model for the pearlitic transformation, are given in (Pietrzyk and Kuziak, 2004).

A rule of mixture is used to describe the flow stress for two-phase materials. The flow stress of mixture σ is:

$$\sigma = \sigma_f f_f + \sigma_a f_a, \quad (21)$$

where f_a and f_f are the volume fractions of phases, while σ_a and σ_f are the flow stresses of austenite and ferrite, respectively.

A finite element solution of the problem defined by (4)–(16), coupled with the solution of the phase transformation model defined by (17) and (18), constitutes the direct problem model in the present work.

2.2. Objective Function

The inverse algorithm described in (Szeliga and Pietrzyk, 2002) for rheological models and in (Kondek *et al.*, 2003) for phase transformation models is used in the present work. The objective of the optimization is the determination of the following parameters:

1. Parameters in the phase transformation model (for the ferritic transformation these are coefficients in (17)–(20)). The objective function is defined as

$$\Phi = \sqrt{\frac{1}{n} \sum_{i=1}^n \left(\frac{T_{im} - T_{ic}}{T_{im}} \right)^2 + \frac{1}{k} \sum_{i=1}^k \left(\frac{f_{im} - f_{ic}}{f_{im}} \right)^2}, \quad (22)$$

where T_{im} and T_{ic} are the measured and calculated temperatures at the beginning and the end of transformations, n is the number of temperature measurements, f_{im} and f_{ic} are the measured and calculated volume fractions of phases in the room temperature, and k is the number of the measurements of volume fractions of phases.

2. Rheological parameters m , n , R_0 , K_0 , K_{sat} , β_{sat} , β in (10) for ferrite and α , A_0 , A_1 , k_{20} , A_{30} , Q_s , Q_m in the internal variable model for austenite. The objective function is defined as

$$\Phi = \sqrt{\frac{1}{Nt} \sum_{i=1}^{Nt} \left[\frac{1}{Npl_i} \sum_{j=1}^{Npl_i} \left(\frac{F_{ij}^c - F_{ij}^m}{F_{ij}^m} \right)^2 \right]}, \quad (23)$$

where F^c and F^m are loads calculated by the direct model and measured in the experiment, Nt is the number of experiments, and Npl_i is the number of sampling points in the i -th experiment.

2.3. Optimization Techniques

The following methods were used in the search for minima of the objective functions:

- Evolutionary algorithm with an automatic adaptation of the resolution of the encoding applied to individual parameters,
- Hooke-Jeeves method with a non-deterministic selection of the order of the search directions in the trial step,
- Nelder and Mead's simplex method,
- Conjugate gradient method based on the Polak-Ribière formulation,
- Variable-metric method (also known as the quasi-Newton method).

Table 1. Values of increments used in a numerical calculation of gradient components of the objective function.

ΔK_0	Δn	$\Delta \beta$	ΔK_s
1e-3	1e-5	1e-5	1e-4
$\Delta \beta_s$	Δm	ΔR_0	
0.5	1e-5	1e-3	

A numerical calculation of the derivatives of the objective function was used in all gradient methods. The mesh of the applied increments is presented in Table 1. The following methods were applied to searching along the selected direction:

- modified direct Brent method,
- modified Brent method based on the magnitude of the gradient,
- backtracking method, which determines the solution iteratively, checking whether it is better than the previous one; this method cannot be considered as an efficient optimization method.

2.4. Experiment

All experiments were carried out at the Institute for Ferrous Metallurgy in Gliwice, Poland. Since carbon-manganese steel was investigated in an earlier research work (Szeliga *et al.*, 2003) and the results were promising, a more complex material, i.e. niobium microalloyed steel, was tested in the present work. Two kinds of tests were performed:

1. Dilatometric tests with cooling rates between 0.04°C/s and 77°C/s . The objective of these tests was to identify the coefficients in the phase transformation model, cf. (17)–(20).
2. Plastometric tests for axisymmetrical samples at temperatures between 550°C and 1100°C , step 50°C and at strain rates 0.1 s^{-1} , 1 s^{-1} and 10 s^{-1} . The objective of these tests was to identify the coefficients in the rheological model, cf. (10)–(16).

An inverse analysis was used for interpreting the results of both types of tests.

3. Results

The optimization problem concerns two models: the rheological model and the phase transformation model. Due to frequent local minima, a genetic algorithm was used

Table 2. Optimized coefficients in (10), which describe the flow stress for ferrite.

a_1	a_2	a_3	a_4	a_5	a_6
2.2	91.4	2.7	460	0.8	0.0

for the identification of coefficients in the former model. The simplex, Hooke-Jeeves and Rosenbrock derivative-free methods were introduced at the final stage of the search. The identification results are shown in Table 2 and Fig. 1. The so-called CTT diagrams, measured and calculated, which represent the start and end temperatures of transformations, are presented in this figure, where F_s is the ferrite start, P_s is the pearlite start and P_f is the pearlite finish. A quite good agreement between measurements and predictions is observed, which confirms identification capabilities of the inverse analysis.

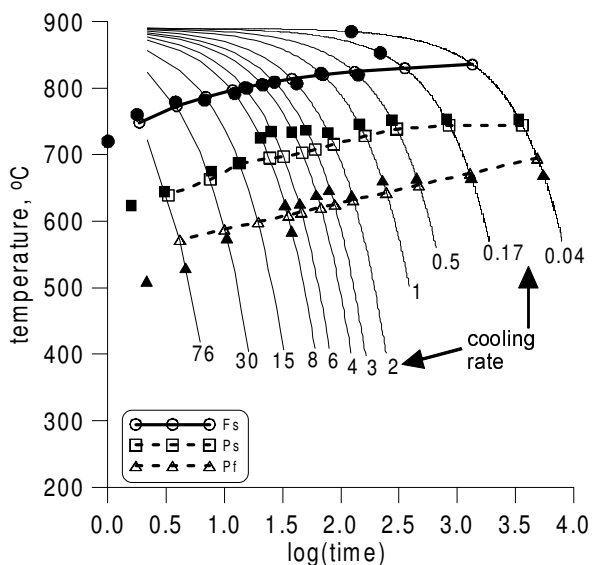


Fig. 1. Comparison of the start and end temperatures of transformations measured in dilatometric tests (discs) and predicted by the model with optimized coefficients (open circles).

The inverse analysis of plastometric tests is based on finite-element simulations and thus the costs of computations are very high. Several (at least nine in the analysed case) finite-element simulations are required to determine one value of the objective function. Thus, the two-step algorithm proposed in (Szeliga and Pietrzyk, 2001) was applied. Each experiment is investigated separately in the first step of the analysis and a solution close to the global minimum is obtained reasonably fast. This step, which is not discussed in detail in this paper, provides a starting point for the final inverse analysis, which is performed using the derivative-free simplex method.

Table 3. Optimized coefficients in (10), which describe the flow stress for ferrite.

K_0	β	m	n	K_{sat}	β_{sat}	R_0
13.1	0.047	0.084	0.079	1.775	3671	19.98

Table 4. Optimized coefficients in the internal variable model (cf. (11)–(16), which describe the flow stress for austenite.

α	A_0	A_1	k_{20}	A_{30}	Q_s	Q_m
1	1.45×10^{-3}	0.16	176	1.97×10^{-10}	34.1	390.5

The development of the best optimization strategy for the inverse analysis was one of the objectives of this work. Therefore, alternatively, a hybrid algorithm, which combines genetic algorithms with local-search methods, was used.

Figure 2 shows a typical example of the comparison between loads measured and predicted using the finite-element code with the constitutive law based on the optimized coefficients. The values of these coefficients for the function (10), which is adequate for the ferritic range of temperatures 550–700°C, are given in Table 3. The coefficients for the internal variable model adequate for the austenitic range of temperatures 850–1100°C are given in Table 4.

It is seen in this figure that the reversed dependence of loads on temperature (loads increase as temperature increases) appears in the transformation range of temperatures. Figure 3, which shows the dependence of the flow stress at the strain 0.4 on temperature, explains better the reasons for this phenomenon. It is seen that for the temperature range 750–800°C the flow stress increases with increasing temperature. This phenomenon is observed for all strain rates.

4. Optimization Strategy

The results presented in Figs. 1 and 2 show that the inverse analysis is an efficient tool for the identification of material models. Having in mind the fact that the model describes the behaviour of a material in a wide range of temperatures (550–1100°C) and strain rates (0.1–10 s⁻¹), including the phase transformation range, the accuracy obtained in Fig. 2 can be considered as good. The authors' experience in the field of the inverse analysis leads to a conclusion that the choice of the optimization method and the starting point for the analysis often presents difficulties. Thus, the general objective of the present work was to suggest the best optimization strategy for the inverse analysis. Therefore, several strategies were tested during

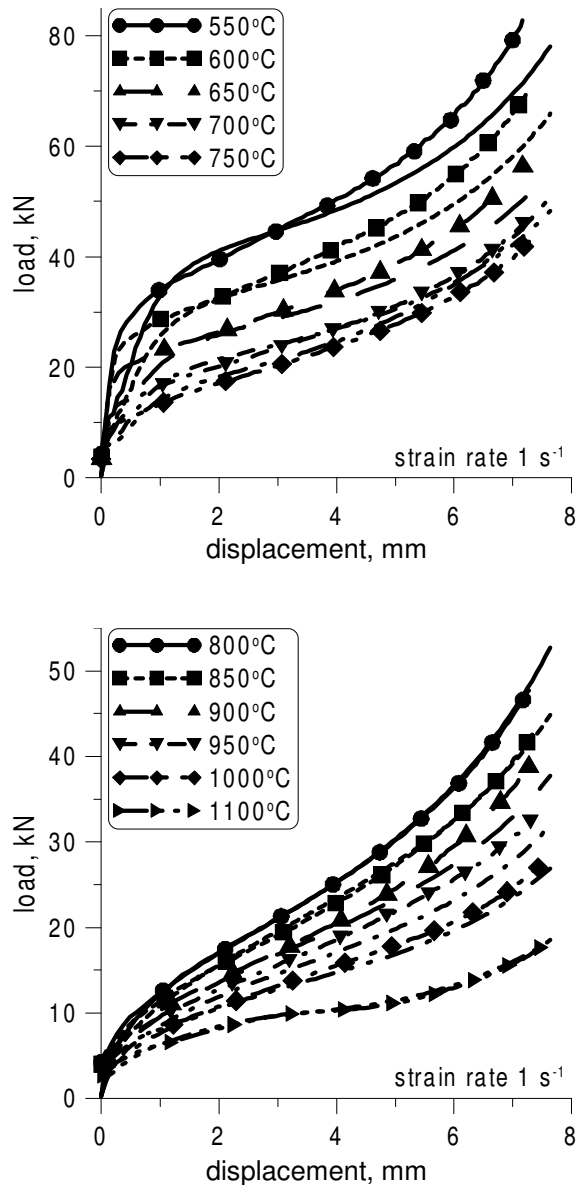


Fig. 2. Loads measured and calculated by the FEM code and the two-phase material constitutive law and optimized coefficients.

the inverse calculations described in the previous sections. The observations from these tests are presented below.

The simulation of the phase transformation using (17)–(20) is fast. Therefore, the computation time is not that important in this case. Avoiding the local minima in the objective function (22) becomes a major problem. What is more, the objective function (23) is smoother but the computational cost of this function evaluation is very high. These aspects have to be accounted for in the choice of the optimization strategy.

Figures 4–5 show the relation between the objective function and the number of runs of the finite-element code

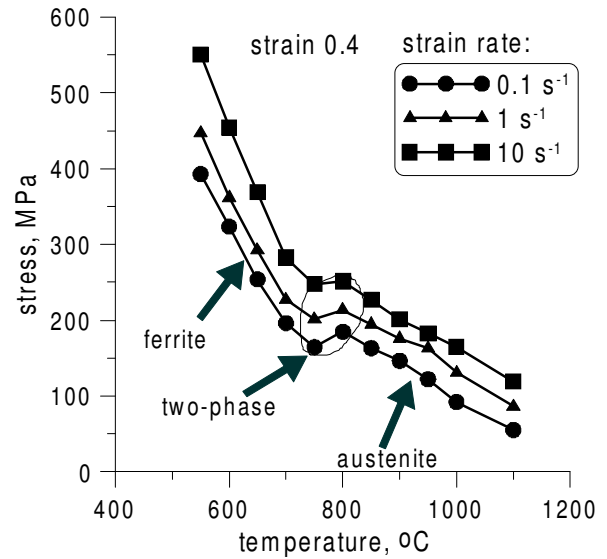


Fig. 3. Flow stress dependence on temperature for the strain of 0.4.

for various optimization techniques. The simplex method was efficient in searching for a minimum and, within reasonable limits, was insensitive to a starting point. The Hooke-Jeeves algorithm and gradient methods achieved satisfactory convergence for the starting points generated earlier either by a genetic algorithm or by the simplex method.

In most cases, the convergence of derivative-free methods was satisfactory whenever the starting point was generated randomly within certain limits or preselected by the genetic algorithm. Figure 5 shows that the conjugate gradient method applied to a starting point obtained from the simplex method leads to a better approximation of the minimum but the improvement is negligible and does not justify additional computation costs.

5. Discussion

A selected example of applying optimization techniques in the inverse analysis has been described. In their previous works, the authors applied the inverse algorithm to interpret various plastometric tests and to identify material and friction models based on the results of these tests. The conclusions below are based on the results of earlier research and on the tests performed in the present work. The latter dealt with the deformation of niobium microalloyed steel in a two-phase region of temperatures (Pietrzyk and Kuziak, 2004).

In consequence, the optimization strategy for the inverse analysis was formulated in two versions:

- When phase transformation models are identified, the computation cost for the evaluation of the objec-

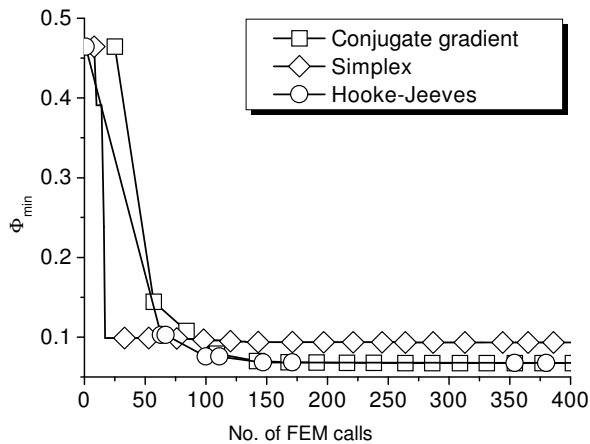


Fig. 4. Comparison of convergence for the conjugate gradient, simplex and Hooke-Jeeves methods as a function of runs of the finite-element code.

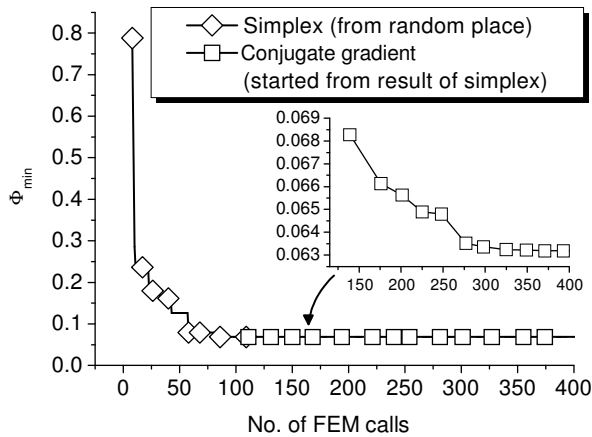


Fig. 5. Changes in the objective function when the simplex method is followed by the conjugate gradient method. The coomed chart shows the results of the conjugate gradient method.

tive function (22) is low. Therefore, genetic algorithms proved to be an efficient tool. In some cases, final optimization can be performed using the simplex method.

- The computation cost for the evaluation of the objective function (23) is very high. Therefore, the hybrid algorithm is suggested for the identification of friction and rheological models. This algorithm involves evolutionary methods at the primary stage of optimization. Due to a very long computation time, parallel computations are advised at this stage. Evolutionary methods are followed either by the simplex method or by gradient methods. There is no clearly defined rule for choosing from these methods. This selection depends on the type of the flow stress function and the number of optimization variables. A

trial-and-error approach is often necessary. Therefore, the inverse user friendly computer program has been developed in (Kondek *et al.*, 2003). This program allows an easy selection of the optimization method for the inverse analysis of compression tests.

The performed analysis yields some observations regarding the advantages of various methods as far as their applicability to the inverse analysis is considered.

Genetic algorithms. *Advantages:* They explore a wide search domain, the objective function can be irregular, and they do not require a starting point. Moreover, they are insensitive to the problem of long valleys. They are easily adapted to parallel computations. *Disadvantages:* large computation costs and the necessity of defining limits for optimization variables.

Derivative-free methods (Hooke-Jeeves, simplex, Rosenbrock). *Advantages:* They explore a wide search domain, the objective function can be irregular, and the simplex method is almost insensitive to the problem of long valleys. *Disadvantages:* A starting point is required, convergence is relatively slow, and the Hooke-Jeeves and Rosenbrock methods are sensitive to the problem of long valleys.

Gradient methods (conjugate gradients, variable metric). *Advantages:* Fast convergence, a more accurate solution compared with genetic algorithms and derivative-free methods. *Disadvantages:* They require a starting point, converge to the nearest local minimum, the objective function has to be regular, problems with determining the gradient of the objective function are encountered, and they are sensitive to the problem of long valleys.

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