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DESCRIPTION OF VISCOPLASTIC FLOW ACCOUNTING FOR SHEAR BANDING

OPIS LEPKOPLASTYCZNEGO PŁYNIĘCIA Z UDZIAŁEM PASM ŚCINANIA

The subject of the study is concerned with ultra fine grained (ufg) and nanocrystalline metals (nc-metals). Experimental investigations of the behaviour of such materials under quasistatic as well as dynamic loading conditions related with microscopic observations show that in many cases the dominant mechanism of plastic strain is multiscale development of shear deformation modes – called shear banding. The comprehensive discussion of these phenomena in ufg and nc-metals is given in [1], [2] and [3], where it has been shown that the deformation mode of nanocrystalline materials changes as the grain size decreases into the ultrafine region. For smaller grain sizes (d < 300 nm) shear band development occurs immediately after the onset of plastic flow. Significant strain-rate dependence of the flow stress, particularly at high strain rates was also emphasized. Our objective is to propose a new description of viscoplastic deformation, which accounts for the observed shear banding. Viscoplasticity model proposed earlier by Perzyna [4], [5] was extended in order to describe the shear banding contribution. The shear banding contribution function, which was introduced formerly by Pęcherski [6], [7] and applied in continuum plasticity accounting for shear banding in [8] and [9] as well as in [10] and [11] plays pivotal role in the viscoplasticity model. The derived constitutive equations were identified and verified with application of experimental data provided in paper [2], where quasistatic and dynamic compression tests of ufg and nanocrystalline iron specimens of a wide range of mean grain size were reported. The possibilities of the application of the proposed description for other ufg and nc-metals are discussed.

Keywords: viscoplastic flow, shear banding, micro-shear bands, nanocrystalline metals, nc-metals, ultra fine grain (ufg) metals

Przedmiotem studiów są drobnoziarniste oraz nanokrystaliczne metale. Badania doświadczalne zachowania się takich materiałów w warunkach obciążeń quasistatycznych oraz dynamicznych, w powiązaniu z obserwacjami mikroskopowymi, wykazują, że w wielu wypadkach dominującym mechanizmem odkształcenia plastycznego jest wieloskalowy rozwój form ścinania – zwany zwojem pasmami ścinania. Wyczerpująca dyskusja tych zjawisk zawarta jest w [1], [2] i [3], gdzie wykazano, że forma odkształcenia w materiałach drobnoziarnistych zmienia się, kiedy rozpatrujemy materiały o coraz mniejszym ziarnie. Dla materiałów o średniej wielkości ziarna mniejszej niż 300 nm obserwuje się rozwój pasm ścinania zaraz po inicjacji odkształcenia plastycznego. Podkreślono także znaczący wpływ prędkości odkształcenia na naprężenie płynięcia. Naszym celem jest propozycja nowego opisu odkształcenia lepkoplastycznego, w którym uwzględnia się udział obserwowanego rozwoju pasm ścinania. Model lepkoplastyczności proponowany wcześniej przez Perzynę [4], [5] został rozszerzony z wykorzystaniem opisu udziału pasm ścinania. Podstawową rolę w proponowanym modelu lepkoplastyczności odgrywa funkcja udziału pasm ścinania wprowadzona przez Pęcherskiego [6], [7] i zastosowana w kontynualnej teorii plastyczności z udziałem pasm ścinania w [8] i [9] oraz w [10] i [11]. Dokonano identyfikacji oraz weryfikacji wyprowadzonych równań konstytutywnych z zastosowaniem danych doświadczalnych otrzymanych w testach quasistatycznego i dynamicznego ściskania dla serii próbek wykonanych z drobnoziarnistego i nanokrystalicznego żelaza o szerokim zakresie średniej wielkości ziarna [2]. Przedyskutowano możliwości zastosowania proponowanego opisu do innych metali o budowie drobnoziarnistej i nanokrystalicznej.

1. Introduction

The subject of our study is concerned with ultra fine grained (ufg) and nanocrystalline metals (nc-metals). Experimental investigations discussed e.g. by Meyers et al. [1] and Jia et al. [2] reveal that nanocrystalline materials exhibit very high yield strength, presumably due to the grain-boundary strengthening known as the Hall-Petch effect. This is generally true at least to the grain sizes, which are not smaller as the tenth of nanometer. The diminishing grain size leads to the situation that dislocation controlled mechanisms of inelastic deformation become hindered and new dislocation-less mechanisms are activated. Then different kinds of grain

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boundary accommodation [1] and shear banding [1], [2], [3] are reported. Experimental investigations of the behaviour of such materials under quasistatic as well as dynamic loading conditions related with microscopic observations show that in many cases the dominant mechanism of plastic strain is multiscale development of shear deformation modes – called shear banding. The comprehensive discussion of these phenomena in ufg and nc-metals is given in [1], [2] and [3], where it has been shown that the deformation mode of nanocrystalline materials changes as the grain size decreases into the ultrafine region. Regarding nc-Fe [2], for smaller grain sizes (d < 300 nm) shear band development occurs immediately after the onset of plastic flow. Significant strain-rate dependence of the flow stress, particularly at high strain rates was also emphasized.

The aim of the paper is to propose a new description of viscoplastic deformation, which accounts for the observed shear banding phenomena. Viscoplasticity model with an overstress function proposed earlier by Perzyna [4], [5] was extended in order to describe the new mechanism of inelastic deformation. The theoretical description of multiscale hierarchy of shear localization modes presented formerly by Pęcherski in [6], [7], [8] and the new concept of shear banding contribution function in the rate of plastic deformation applied in continuum plasticity accounting for shear banding in [6], [8] , [9], [11] and identified for polycrystalline Cu in [10] and [12] plays pivotal role in the viscoplasticity model. The derived constitutive equations were identified and verified with application of experimental data of quasistatic and dynamic compression tests, made for a wide range of ufg and nanocrystalline iron specimens of different mean grain size, which were provided in [2]. The possibilities of the application of the proposed description for other ufg and nc-metals are discussed. Although constitutive modelling of strength and inelastic behaviour of nanomaterials is still at the beginning of its development, some attempts to propose constitutive description can be mentioned. For example, in [13] grain boundary mechanisms are emphasized and a Taylor-type phase mixture model was proposed for calculation of stress to describe the deformation behaviour of a nanocrystalline metallic materials. In [14] another constitutive model for nanocrystalline metals was derived, in which a cooperative grain boundary mechanisms play crucial role. The main assumption is made that plastic deformation is accommodated at the primarily grain boundaries and the insertion and rotation processes are considered together as a cooperative deformation mechanisms. The paper provides the overview of earlier attempts in accounting for grain boundary mechanisms. The paper [15] presents, on the other hand, a phenomenological approach, modifying the proposed earlier viscoplastic model by including a bi-linear Hall-Petch type relation to correlate with the response of nanocrystalline aluminum and iron. Recently, a viscoplastic micromechanical models for the yield strength of nanocrystalline materials were derived in [16], [17] and [18]. It was emphasized in [16] that when the grain dimensions approach nanometre sizes, the volume fractions of grain boundaries increase the grain boundary regions and start to play an active role in accommodating deformation. The grain boundary accommodation may involve local shuffling of atoms, grain boundary sliding and different diffusive processes. Also pressure and grain size dependency of yield strength were discussed. The papers [17] and [18] are devoted to theoretical description and computational analysis of inelastic deformation of powder-processed nc-metals. The detail analysis of micromechanical mechanisms controlling inelastic behaviour of material can give physical motivation for our description based on two mechanisms of viscoplastic flow: dislocation controlled slips and shear banding.

2. Constitutive modelling

The viscoplasticity flow law proposed by Perzyna [4], [5] is applied

$$\mathbf{D}^{vp} = \frac{\sqrt{2}}{2}\dot{\gamma}_s^{vp}\boldsymbol{\mu}, \qquad \boldsymbol{\mu} = \frac{1}{\sqrt{2}k_s}\boldsymbol{\tau}', \tag{2.1}$$

$$\dot{\gamma}_s^{vp} = \dot{\gamma}_0\left[\frac{J_2}{k_s} - 1\right]^{\frac{1}{D}} \quad \text{for} \quad J_2 - k_s > 0\ , \quad J_2 = \sqrt{\frac{1}{2}\boldsymbol{\tau}' : \boldsymbol{\tau}'} \tag{2.2}$$

and

$$\dot{\gamma}_s^{vp} = 0 \quad \text{for} \quad J_2 - k_s \leqslant 0\ , \tag{2.3}$$

where $\mathbf{D}^{vp}$ is the rate of viscoplastic deformation, $\boldsymbol{\tau}'$ denotes deviatoric Kirchhoff stress and $\dot{\gamma}_s^{vp}$ is the viscoplastic shear strain rate produced by the mechanism of dislocation mediated crystallographic slips, while k_s is the corresponding quasistatic yield shear strength. The symbols $\dot{\gamma}_0$ and D denote material constants. The shear strain rate (2.2) is controlled by an overstress function to be specified for a particular material. In our case the power-like overstress function is assumed.

It is well known fact that in nc-metals, in particular if they are powder consolidated, plastic flow is in general pressure dependent, plastically dilatant and non-normal, cf. e.g. [18]. An attempt to apply the Burzyński yield condition accounting for pressure sensitivity and strength differential effect was presented in [19] and

[20], cf. also the forthcoming paper [21]. The quasistatic Huber-Mises yield condition $\boldsymbol{\tau}' : \boldsymbol{\tau}' = 2k_s^2$ is assumed here for simplicity as a first approximation. This is more suitable for ufg and nc-metals manufactured with application of severe plastic deformation processes. The results of the derived description of the quasistatic and dynamic flow stress can be applied for different loading paths and general stress states with use of the Burzyński yield condition [21]. In derivation of viscoplasticity flow law for ufg and nc-metals, the assumption of the operation of two mechanisms: dislocation mediated crystallographic slips in the crystalline grain interiors and shear banding in the intercrystalline grain-boundary regions play pivotal role. The contribution of both mechanisms in the rate of plastic deformation was studied earlier by Pęcherski in [6], [7], [8] and [9] where the process of shear banding was idealized mathematically as a hierarchy of singular surfaces. The singular surface of order zero corresponds to the local perturbation of the microscopic displacement field produced by the passage of a single micro-shear band. The passage of large number of micro-shear bands within the active zone of the cluster, which the micro-shear bands form, smoothes out the discontinuity on the micro-level and results in the perturbation of the mezoscopic displacement field traveling with the speed V_s, which produces a discontinuity of the mezoscopic velocity filed $\mathbf{v}_M$ in the RVE it traverses. This corresponds to the singular surface of order one, called also the surface of strong discontinuity. According to [22] and [23], the surface of strong discontinuity of velocity field fulfills the properties of a vortex sheet with the jump discontinuity $[\mathbf{v}_M] = V_s\, \mathbf{s}$, where $\mathbf{s}$ is the unit tangent to the discontinuity surface [7]. An extension of the known averaging procedure over the RVE traversed by a strong discontinuity surface led to the macroscopic measure of velocity gradient produced in the course of elastic-plastic deformation accounting for shear banding. As it was mentioned in [11], the progression of large number of clusters of micro-shear bands extending the region of shear banding can be idealized mathematically by means of the singular surface of order two propagating through the macro-element of the continuum as an acceleration wave. The application of the theory of stationary acceleration waves opens the possibility of the analysis of plastic flow instabilities in relation with shear banding. As a result of the mentioned above studies the following additive decomposition of the rate of inelastic deformation was obtained:

$$\mathbf{D}^{vp} = \mathbf{D}_s^{vp} + \mathbf{D}_{SB}^{vp} \tag{2.4}$$

and the scalar shear banding contribution function was defined:

$$f_{SB} = \frac{\left\|\mathbf{D}_{SB}^{vp}\right\|}{\left\|\mathbf{D}^{vp}\right\|}\ , \quad \|\mathbf{A}\| = \sqrt{\mathbf{A}\cdot\mathbf{A}} = \sqrt{A_{ij}A_{ij}}, \tag{2.5}$$

where $\mathbf{A}$ is a symmetric second order tensor, while $\mathbf{D}_s^{vp}$ is the rate of viscoplastic deformation produced by dislocation mediated crystallographic slips and $\mathbf{D}_{SB}^{vp}$ denotes the rate of viscoplastic deformation produced by shear banding. As discussed in [11], among many possible realizations of shear banding, one can single out the group of processes characterizing with the same contribution of two symmetric shear banding systems $f_{SB}^{(1)} = f_{SB}^{(2)}$. In the case of proportional loading paths the total viscoplastic shear strain rate can be expressed as follows:

$$\dot{\gamma}^{vp} = \dot{\gamma}_s^{vp} + \dot{\gamma}_{SB}^{vp} \tag{2.6}$$

and due to $f_{SB} = \frac{\dot{\gamma}_{SB}^{vp}}{\dot{\gamma}^{vp}}$ we have

$$\dot{\gamma}^{vp}(1 - f_{SB}) = \dot{\gamma}_s^{vp}\ \ ,\ \ f_{SB} \in [0, 1)\ , \tag{2.7}$$

what leads according to (2.2) to the following constitutive relation for the viscoplastic shear strain rate controlled by the discussed mechanisms of crystallographic slip and shear banding:

$$\dot{\gamma}^{vp} = \frac{\dot{\gamma}_0^{vp}}{(1 - f_{SB})}\left[\frac{J_2}{k_s} - 1\right]^{\frac{1}{D}} \quad \text{for} \quad J_2 - k_s > 0\ . \tag{2.8}$$

Inverting (2.8) gives the relation for the dynamic yield condition

$$J_2 = k_s^d = k_s\left\{1 + \left[\left(\frac{\dot{\gamma}^{vp}\,(1 - f_{SB})}{\dot{\gamma}_0}\right)^D\right]\right\}. \tag{2.9}$$

In the forthcoming paper [24] the relation for the dynamic yield shear strength k_d was derived for the RVE in which the mechanisms of crystallographic slip and shear banding are operative. The derivation is based on the balance of the sum of the rate of dissipation produced by each mechanism and the rate of dissipation of the deformation of whole RVE. It is under assumption that the material reveals no work hardening. It is also assumed that the value of the threshold stress of shear banding is negligible in comparison with the value of k_s^d. As a result, the following relation was obtained:

$$k_d = (1 - f_{SB})\left(1 - f_{SB}^V\right)k_s^d\ , \tag{2.10}$$

where $f_{SB}^V = \frac{V_{SB}}{V}$ is the volume fraction of the region of RVE in which shear banding mechanism operates. Assuming that $f_{SB} \approx f_{SB}^V$, the relation (2.10) reads

$$k_d = (1 - f_{SB})^2 \, k_s^d \ , \qquad (2.11)$$

and consequently we have

$$k_d = (1 - f_{SB})^2 \, k_s \left\{ 1 + \left[\left(\frac{\dot{\gamma}^{vp} \, (1 - f_{SB})}{\dot{\gamma}_0} \right)^D \right] \right\} . \qquad (2.12)$$

For the compression test considered in [2] the following specification of quasistatic yield strength can be proposed

$$\sigma_{Ys} = A(d) + B(d)(\varepsilon^{vp})^n \ , \qquad (2.13)$$

where $\sigma_{Ys} = \sqrt{3} k_s$ and ε^{vp} is the equivalent plastic strain $\varepsilon^{vp} = \frac{\sqrt{3}}{3}\gamma^{vp}$. The final relation for the dynamic yield strength in uniaxial compression test takes the form

$$\begin{aligned} \sigma_{Yd} = \ & (1 - f_{SB})^2 \ [A(d) + B(d)(\varepsilon^{vp})^n] \\ & \left[1 + \left(\frac{(1 - f_{SB}(d)) \ \dot{\varepsilon}^{vp}}{\dot{\varepsilon}_0(d)} \right)^D \right] . \end{aligned} \qquad (2.14)$$

The symbol $A(d)$ denotes the quasistatic initial yield strength depending on mean grain diameter d, e.g. according to Hall-Petch relation and n corresponds to plastic hardening parameter. Furthermore, the viscosity parameter $\dot{\varepsilon}^0$ and the contribution function f_{SB} are assumed to be dependent on the mean grain diameter d.

The shape of the contribution function f_{SB} is proposed, accounting to the studies in [8] and [10] supported by the numerical identification and verification in [12], in the form of logistic function:

$$f_{SB} = \frac{f_{SB_0}}{1 + \exp(a - b(d)\varepsilon^{vp})} \ , \qquad (2.15)$$

where $f_{SB_0}, a, b(d)$ are material parameters to be specified.

The proposed specification of the contribution function f_{SB} is suitable for the description of proportional loading processes. More general formula, applicable for arbitrary states of deformation and loading paths, was proposed in [25] and analysed in [26].

3. Identification of the model parameters

The basic idea of the identification procedure was to determine all material constants without the use of numerical simulations. This was found possible using a direct curve fit to given experimental data, assuming proportional straining and constant strain-rate. The method of least squares requires the residual sum in stress between the experimental observations and model results to be minimised. This implies that the proposed model of rate dependent plasticity can be completely calibrated by minimising the residual function:

$$\begin{aligned} F(x) = \min \sum_{\alpha=1}^{N_\alpha} \cdot \\ \cdot \left\{ \sigma_{eq}^{\exp} \left(\varepsilon_\alpha^{vp}, \ \dot{\varepsilon}^{vp}, \ d \right) - \sigma_{eq}^{cal} \left(\varepsilon_\alpha^{vp}, \ \dot{\varepsilon}^{vp}, \ d, \beta \right) \right\}^2 \end{aligned} \qquad (3.16)$$

where $F(x)$ refers to the residual of the constitutive model and the experimental data with $\beta = (a, b, f_{SB_0}, A, B, n, \dot{\varepsilon}_0^p, D)$ and β denotes a vector of unknown material parameters to be determined.

Furthermore, ε_α^{vp} are discrete values of the strains ε^{vp}. The symbols $\sigma_{eq}^{\exp}$ and σ_{eq}^{cal} denote the experimental and calculated stresses for the same strain level ε_α^{vp}, N_α is the number of stress-strain data for the test with given strain rate and grain size. For our constitutive equation (2.14) accounting for (2.15) we have

$$\sigma_{eq}^{cal} = \sigma_{Yd} = \left(1 - \frac{f_{SB_0}}{1+\exp(a - b(d)\varepsilon_\alpha^{vp})} \right)^2 \cdot$$

$$\left(A(d) + B(d)(\varepsilon_\alpha^{vp})^n \right) \cdot \left(1 + \left(\frac{\left(1 - \frac{f_{SB_0}}{1+\exp\left(a \ - \ b\left(d\right)\varepsilon_\alpha^{vp}\right)} \right) \dot{\varepsilon}_\alpha^{vp}}{\dot{\varepsilon}_0^{vp}(d)} \right)^D \right) . \qquad (3.17)$$

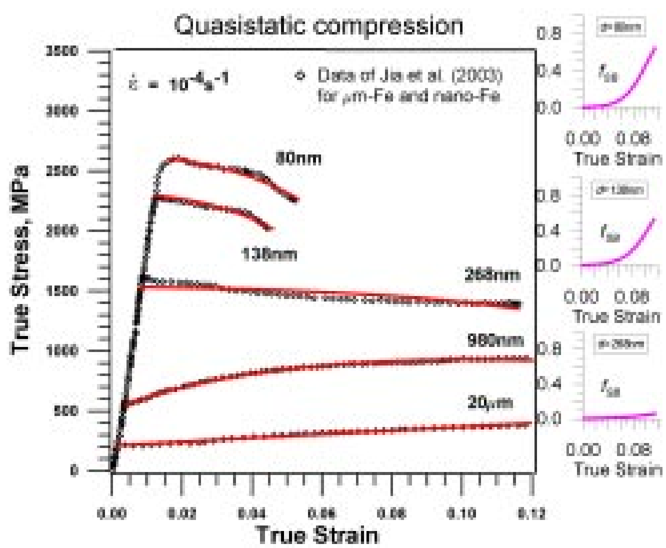

Fig. 1. True stress – true strain for quasistatic compression test for polycrystalline iron of purity 99.9% obtained in two-step consolidation procedure to form bulk Fe with desired grain size [2]. Solid lines represent curves obtained from viscoplasticity model accounting for shear banding according to equations (3.18) and (3.19), symbols ⋄ correspond to experimental data from [2]. On the right hand side the plots of f_{SB} – true strain for corresponding three mean grain diameters d, are displayed

An example of the application of the proposed constitutive description for modelling of the behaviour of polycrystalline iron under quasistatic and dynamic compression tests for experimental data of Jia, Ramesh and Ma (2003) is depicted in Fig. 1 and Fig. 2 (cf. [2]).

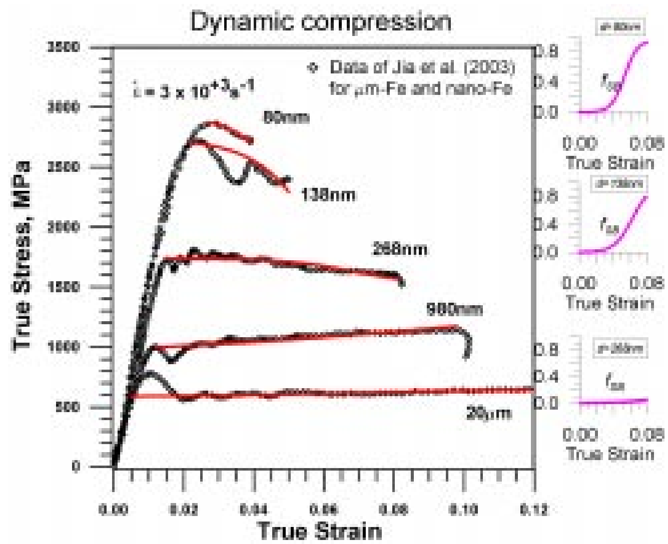

Fig. 2. True stress – true strain for dynamic compression test for polycrystalline iron of purity 99.9% obtained in two-step consolidation procedure to form bulk Fe with desired grain size [2]. Solid lines represent curves obtained from viscoplasticity model accounting for shear banding according to equations (3.18) and (3.19), symbols ⋄ correspond to the dynamic experimental data from [2]. On the right hand side the plots of f_{SB} – true strain for corresponding three mean grain diameters d, are displayed

In the case of quasistatic and dynamic compression we use the following forms of equation (3.17):
when $d > 300$ nm, $f_{SB} = 0$, $n = 0.2$, $\dot{\varepsilon}_0(d) = 0.3 \cdot 10^{+2} s^{-1}$ and $D = 0.08$

$$\sigma_{eq}^{cal} = \left[A(d) + B(d)(\varepsilon_\alpha^{vp})^n\right] \left[1 + \left(\frac{\dot{\varepsilon}^{vp}}{\dot{\varepsilon}_0(d)}\right)^D\right], \quad (3.18)$$

and when $d < 300$ nm, $0 < f_{SB} < 1$, $n = 0$, $B = 0$, $D = 0.08$, $a = 5.0$ and $f_{SB_0} = 0.95$

$$\sigma_{eq}^{cal} = \left(1 - \frac{f_{SB_0}}{1 + \exp\left(a - b(d)\varepsilon_\alpha^{vp}\right)}\right)^2 [A^*(d)] \left[1 + \left(\frac{\left(1 - \frac{f_{SB_0}}{1+\exp\left(a - b(d)\varepsilon_\alpha^{vp}\right)}\right)\dot{\varepsilon}^{vp}}{\dot{\varepsilon}_0(d)}\right)^D\right]. \quad (3.19)$$

The following constitutive parameters are found with a nonlinear least squares fit:

TABLE 1

Grain size d	$A(d)$ or $A^*(d)$ [MPa]		$B(d)$ [MPa]	$b(d)$	
	quasistatic	dynamic		quasistatic	dynamic
80 nm	**1920.0**	**1205.0**	**–**	**77.66**	**98.28**
138 nm	**1740.0**	**1120.0**	**–**	**77.34**	**94.95**
268 nm	**1160.0**	**710.0**	**–**	**22.64**	**28.59**
980 nm	**277.96**	**106.78**	**602.25**	**–**	**–**
20μm	**76.14**	**100.28**	**269.41**	**–**	**–**

4. Conclusions

This paper presents the description of rate-dependent plastic behaviour of usg and nc-metals. The new feature of our proposition is account for shear banding. The mechanisms of multiscale shear band formation are responsible for accommodation of inelastic deformation of material if only dislocation controlled mechanisms become hindered. Therefore, the proposed description can also be applied for other ufg, nc-metals as well as for different kinds of hard-deformable materials.

The identification of constitutive relations of viscoplastic flow was made locally for a material point. This is based on rather crude assumption that during the observed processes of compression the investigated material behaves homogeneously in the whole sample. More adequate analysis requires the inverse solution of the boundary value problem simulating numerically the compression test process. The derived constitutive equations will be applied for solution of such an inverse problem as well as for verification with use of other independent experimental test.

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