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A method of determination of inelastic constitutive equations (*)

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To DETERMINE a sufficiently accurate, concrete form of constitutive equation for a given inelastic material seems to be most critical problem of inelasticity at present. In the suggested method a corresponding inverse problem is formulated and solved. The method is illustrated with an example where information gained from a series of tensile tests suffices to solve the inverse problem. The inelastic constitutive equations for mild steel are derived and used in the solution of the coupled thermoplastic heat conduction problem of torsion of a steel shaft. The predicted torque and surface temperature are compared with the results of the torsion experiment.

Określenie wystarczająco dokładnej i konkretnej postaci równań konstytutywnych dla danego materiału niesprężystego jest w chwili obecnej krytycznym problemem mechaniki ośrodków niesprężystych. W zaproponowanej tu metodzie sformułowano i rozwiązano odpowiedni problem odwrotny. Metodę zilustrowano przykładem, w którym informacja zdobyta z serii doświadczeń na rozciąganie wystarcza do rozwiązania problemu odwrotnego. Wyprowadzone niesprężyste równania konstytutywne dla miękkiej stali zostały zastosowane do rozwiązania sprzężonego zagadnienia termoplastycznego przewodnictwa ciepła w przypadku skręcania stalowego wału. Obliczone moment skręcający i temperatura powierzchniowa zostały porównane z wynikami doświadczeń na skręcanie.

Определение достаточно точного и конкретного вида определяющих уравнений для данного неупругого материала является в настоящий момент критической проблемой механики неупругих сред. В предположенном здесь методе сформилирована и решена соответствующая обратная проблема. Метод иллюстрируется примером, в котором информации полученной из серии испытаний на растяжение хватает для решения обратной проблемы. Выведенные неупругие определяющие уравнения для мягкой стали применены для решения сопряженной термо-пластической задачи теплопроводности в случае скручивания стального вала. Вычисленные скручиваниющий момент и поверхностная температура сравнены с результатами испытаний на скручивание.

1. Introduction

IN RECENT years some effort has been directed to improve the classical theory of thermoplasticity and to formulate a consistent theory of real inelastic materials [1]. The attempts to formulate "improved" theories can be roughly divided in two categories.

One of these attempts is usually called the internal (or hidden) variable approach to thermoplasticity. It is assumed that the present stress-response of the material is determined by the present values of deformation, temperature, and a set of internal variables. The evolution of internal variables is controlled by a system of differential equations.

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[1] The term "inelastic material" is used as a synonym of "temperature sensitive elastic rate-dependent plastic material".

The second approach, which may be called the functional approach, uses the mathematical language of functionals (in practice the functionals usually have a form of integrals) to express the influence of deformation and temperature histories upon the present stress-response.

Both approaches represent a positive step towards a more realistic description of inelastic properties of materials. However, newly formulated theories lose one important feature — the simplicity of the classical theory. The "improved" constitutive equations are more complex. Therefore, it seems that to determine the concrete form of "improved" constitutive equations for a studied material is at present the most critical problem. The problem is essential both for a verification of the correctness of suggested "improved" theories and their use in engineering practice.

The proposed method of determination of inelastic constitutive equations is of a similar nature to that suggestion described at the end of the book by ILIUSHIN [1] or the method used within the framework of classical viscoplasticity by LEMAITER [2]. The proposed method consists of three standard steps:

(i) A sufficiently *general form of inelastic constitutive equations* is assumed at the outset.

(ii) All available special information concerning the studied class of materials and thermo-mechanical processes are used to *restrict the generality of the constitutive equations* adopted in step (i).

(iii) Finally, for the restricted form of the constitutive equations specified by step (ii) we attempt to formulate and solve the corresponding *inverse problem*, i.e. using data from suitably designed experiments, we try to determine the remaining unknown functions to get the concrete form of the constitutive equations in the cases studied.

The steps (i) to (iii) and a preliminary attempt to verify the usefulness of the method will be described in the following sections. A deeper theoretical analysis of the corresponding inverse problem and more detailed experimental verification of the suggested method will be given in a subsequent paper.

2. The assumed general constitutive equations

In the suggested method we shall adopt the internal variable approach to inelasticity (e.g. [3–7]). As the first step of the method we choose one of the possible general forms of inelastic constitutive equations described in detail in [8, 9]:

$$\psi = \tilde{\psi}(\mathbf{C}_E, \theta, \boldsymbol{\alpha}), \tag{2.1}$$

$$h = \mathbf{E}\tilde{\mathbf{h}}(\mathbf{C}_E, \theta, \mathbf{E}^T \operatorname{grad} \theta, \boldsymbol{\alpha}), \tag{2.2}$$

$$\dot{\mathbf{P}}\mathbf{P}^{-1} = \tilde{\mathbf{p}}(\mathbf{C}_E, \theta, \mathbf{E}^T \operatorname{grad} \theta, \boldsymbol{\alpha}), \tag{2.3}$$

$$\dot{\boldsymbol{\alpha}} = \tilde{\mathbf{a}}(\mathbf{C}_E, \theta, \mathbf{E}^T \operatorname{grad} \theta, \boldsymbol{\alpha}), \tag{2.4}$$

where $\mathbf{E}$ and $\mathbf{P}$ are, respectively, elastic and plastic parts of the deformation gradient $\mathbf{F}$, i.e. $\mathbf{F} = \mathbf{EP}$, $\mathbf{C}_E = \mathbf{E}^T \mathbf{E}$ is the right elastic Cauchy-Green tensor, θ denotes temperature, ψ is free energy, and h means the heat flux. The quantity denoted by $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_n)$ describes structural changes in the material during a thermomechanical process (if the structural changes have to be expressed through quantities of higher tensorial rank than scalars, then $\boldsymbol{\alpha}_i$ means the convected quantities with respect to **E**). As a consequence of the second law of thermodynamics ψ does not depend on the temperature gradient [see (2.1)], and Cauchy stress tensor **T** and entropy η are determined through the stress and entropy relations $\mathbf{T} = 2\varrho\, \partial\psi/\partial \mathbf{C}_E$ and $\eta = -\partial\psi/\partial\theta$, ϱ is the mass density.

An infinitesimal strain version of the constitutive equations (2.1)–(2.4) can be reached, if small strain measures $\mathbf{e} = (\mathbf{E}^T\mathbf{E}-\mathbf{1})/2$, $\mathbf{p} = (\mathbf{P}^T\mathbf{P}-\mathbf{1})/2$ are used, and E and P differ only infinitesimally from the unit tensor **1**.

3. The restricted constitutive equations

The second step of the method consists of the specification of all information which is characteristic to the studied class of inelastic materials and thermo-mechanical processes. A representative example of such information is the following list of restrictions:

(a) free energy is a sum of free energy ψ_1 of linear thermoelasticity and energy ψ_2 stored by structural changes of the material;

(b) the heat flux obeys the classical conduction law;

(c) plastic deformation and the structural changes are not influenced by hydrostatic pressure and a temperature gradient;

(d) plastic deformation preserves the volume of the material;

(e) the structural changes can be described by a single scalar parameter;

(f) unstressed states of the material are isotropic.

If we study only quasi-static thermo-mechanical processes the restrictions (a) to (d) are usually satisfied by most materials under standard conditions. The last two assumptions are more restrictive and vary from situation to situation. The degree of isotropy (or type of anisotropy) can be controlled, e.g. by X-ray technique. A hint concerning the number and tensorial character of structural parameters needed in the constitutive equations for the studied class of materials and thermo-mechanical processes can usually be gained from work-hardening theories.

If the restrictions (a) to (f) are expressed in mathematical terms and applied to (2.1) to (2.4) we obtain

$$\psi = \hat{\psi}_1(C_E, \theta) + \hat{\psi}_2(\alpha), \tag{3.1}$$

$$h = -c \operatorname{grad} \theta, \tag{3.2}$$

$$(\dot{\mathbf{P}}\mathbf{P}^{-1})_{\text{sym}} = \hat{d}_1 \mathbf{T}_D + \hat{d}_2 [\mathbf{T}_D^2 - (\operatorname{tr} \mathbf{T}_D^2/3)\mathbf{1}], \tag{3.3}$$

$$\dot{\alpha} = \hat{a}, \tag{3.4}$$

where $\mathbf{T}_D$ means the deviatoric part of **T**, $\mathbf{T}_D = \mathbf{T} - \operatorname{tr}\mathbf{T}/3$, c is heat conductivity, and $\hat{d}_1$, $\hat{d}_2$, $\hat{a}$ are scalar functions of θ, α, and the principal invariants II, III of $\mathbf{T}_D$. The restricted form of the constitutive equations (3.1) and (3.2) is a direct consequence of the restrictions (a) and (b), the relations (3.3) and (3.4) can be obtained from (c) to (f) using the representation theorems for isotropic scalar and tensor functions [10].

The constitutive equations (3.1) to (3.4) will be fully determined, if we are able to find the remaining unknown constitutive functions $\hat{\psi}_1(\mathbf{C}_E, \theta)$, $\hat{\psi}_2(\alpha)$, $\hat{d}_1(\alpha, \theta, \mathrm{II}, \mathrm{III})$, $\hat{d}_2(\alpha, \theta, \mathrm{II}, \mathrm{III})$ and the constant c. The necessary information concerning $\hat{\psi}_1$ and c can easily be obtained from standard tables of elastic constants, specific heat and heat conductivity. If stored energy can be measured (for methods of measurement see [11]) during experiments which will be described in Sec. 4, we have direct information on the second part of free energy ψ_2. To determine $\hat{d}_1$, $\hat{d}_2$, and $\hat{a}$, a corresponding inverse problem has to be solved.

4. Solution of the inverse problem

The unknown constitutive functions $\hat{d}_1$, $\hat{d}_2$, and $\hat{a}$ specify the form of the system of the differential equations (3.3) and (3.4). To determine these functions we need information on the solutions of the Eqs. (3.3) and (3.4) of the same "magnitude" as we are looking for; i.e. we need to know suitable three scalar functions of four scalar variables. Such information can be gained e.g. from biaxial loading experiments combined with measurements of structural changes. Such experiments can yield a set of curves which represent the functions

$$\alpha = \hat{f}(t, \theta, v_1, v_2), \tag{4.1}$$

$$P_1 = \hat{P}_1(t, \theta, v_1, v_2), \quad P_2 = \hat{P}_2(t, \theta, v_1, v_2). \tag{4.2}$$

We suppose in (4.1) and (4.2) that in the biaxial loading experiments two principal components of stress T_1 and T_2 are controlled as a linear function of time t, i.e. $T_1 = v_1 t$, $T_2 = v_2 t$, the third component is kept zero. We measure at various temperatures θ, and loading speeds v_1 and v_2, two principal components of plastic deformation P_1 and P_2 and a quantity sensitive to structural changes α. Following physical metallurgy experience we can measure as α the dislocation density using e.g. etching pits or electron microscope technique. If any macroscopic quantity sufficiently sensitive to structural changes caused by inelastic deformation is available, we would use it as α.

From (4.1) and (3.4) the unknown function $\hat{a}$ can be expressed in the form

$$\hat{a}(\alpha, \theta, \mathrm{II}, \mathrm{III}) = \dot{\alpha} = \frac{\partial}{\partial t}\hat{f}(t, \theta, v_1, v_2), \tag{4.3}$$

where we substitute for $v_1 = T_1/t$, $v_2 = T_2/t$ and $t = g_{\mathrm{inv}}(\alpha, \theta, T_1, T_2)$, inverting the function $\alpha = \hat{f}(t, \theta, T_1/t, T_2/t) \equiv \hat{g}(t, \theta, T_1, T_2)$ with respect to t. Finally, the components T_1 and T_2 have to be expressed in terms of the invariants II and III using $T_1 = 2T_D^{(1)} + T_D^{(2)}$, $T_2 = T_D^{(1)} + 2T_D^{(2)}$, where $T_D^{(1)}$, $T_D^{(2)}$ are roots of $T_D^3 + \mathrm{II}\, T_D + \mathrm{III} = 0$, $T_D^{(3)} = -T_D^{(1)} - T_D^{(2)}$. (An analysis of conditions under which the used operations are possible will be given in a subsequent paper).

Similarly, if $\hat{d}_1$ and $\hat{d}_2$ are evaluated from the Eq. (3.3) written for P_1 and P_2, and (4.2) is used, we get for $i = 1, 2$

$$\hat{d}_i(\alpha, \theta, \mathrm{II}, \mathrm{III}) = \hat{G}_i(T_1, T_2)\hat{F}_1^{-1}\frac{\partial F_1}{\partial t} - \hat{G}_i'(T_1, T_2)\hat{F}_2^{-1}\frac{\partial F_2}{\partial t}, \tag{4.4}$$

where

$$\hat{G}_1 = (2T_2^2-2T_1T_2-T_1^2)/3\Delta, \quad \hat{G}_2 = (2T_1^2-2T_1T_2-T_2^2)/3\Delta,$$

$$\hat{G}'_1 = -(2T_2-T_1)/\Delta, \quad \hat{G}'_2 = -(2T_1-T_2)/\Delta, \quad \Delta = T_1T_2^2-T_1^2T_2, \text{ i.e.}$$

we must have $T_1 \neq 0$, $T_2 \neq 0$, $T_1 \neq T_2$. In F_1 and F_2 the same substitution for v_1, v_2, and t as in the case (4.3) has to be introduced.

Hence, if information specifying (4.1) and (4.2) is available, the solution of the inverse problem (4.3) and (4.4) is reduced to a problem of differentiation and inversion of the functions $\hat{f}$, $\hat{F}_1$, and $\hat{F}_2$. In practice where the relations (4.3) and (4.4) can be obtained only in a form of discrete points and curves the operations of differentiation and inversion have to be combined with interpolation. The concrete constitutive equations are then obtained in the form of tables. The tables can be directly stored in the memory of a computer or we can attempt to approximate the tables by an analytical formula. In the latter case analytical forms of constitutive equations which appear in work-hardening theories may be helpful.

The above discussion indicates that the most difficult point of the method is to perform a sufficient number of accurate experiments which would provide enough information on (4.1) and (4.2). Rough estimate shows the difficulty of the problem. If n measurements suffice to cover a range of variable changes in (4.1) and (4.2) we have to perform n^4 measurements of structural changes and $2n^3$ measurements of deformation curves. In a case of smooth dependences n can be e.g. 5, and to estimate the accuracy of the measurements we need to repeat each measurement at least 4–5 times, i.e. the number of measurements is $5(5^4+2.5^3)$, which is not impossible, but beyond the capacity of an ordinary mechanical laboratory (the number can be substantially decreased using methods of rational planning of experiments, e.g. [12]). From this practical point of view any additional restriction of the type (a) to (f) which reduces the number of unknown constitutive functions and especially the number of their variables is most welcomed. Of course the range of applicability of the derived constitutive equations is then further limited. An example of a further restricted inverse problem will be discussed in the following section.

5. Torsion of steel shaft

In this section for a restricted class of thermo-mechanical processes the concrete form of the constitutive equations for mild steel will be derived and used in the solution of a boundary value problem.

To decrease substantially the number of measurements needed for the solution of the inverse problem, we introduce additionally to (a)–(f) (Sec. 3) the following restrictions:

(g) only undirectional small strain experiments are considered;

(h) temperature is always sufficiently low to exclude aging and recovery effects;

(i) studied thermo-mechanical processes start always at the same initial state of the material;

(j) stored energy ψ_2 can be neglected.

In the small strain range assumed by (g) the dependence of $(\dot{\mathbf{P}}\mathbf{P}^{-1})_{\text{sym}}$ on $\mathbf{T}_D^2$ and the dependence of $\hat{d}_1$ and $\hat{a}$ on III in (3.3) and (3.4) can be neglected. Further, based on the work-hardening theories (e.g. [13, 14]) we can conclude that in the case of thermomechanical processes which respect to (g) and (h) the rate of structural changes is proportional to the rate of plastic deformation; then due to (i) α can be expressed in terms of the invariants of plastic deformation and excluded from explicit consideration. If we use small strain measures $\mathbf{e} = (\mathbf{E}^T\mathbf{E}-\mathbf{1})/2$ and $\mathbf{p} = (\mathbf{P}^T\mathbf{P}-\mathbf{1})/2$ and accept also (j) we can get from (3.1) to (3.4) a further restricted form of the constitutive equations

$$\psi = \bar{\psi}_1(e, \theta), \tag{5.1}$$

$$\mathbf{h} = -c \operatorname{grad} \theta, \tag{5.2}$$

$$\dot{\mathbf{p}} = \bar{d}_1 (\mathrm{II}_P, \theta, \mathrm{II}) \mathbf{T}_D, \tag{5.3}$$

where II_P is the second principle invariant of $\mathbf{p}$ (as a consequence of the restriction (d) $I_p = \operatorname{tr}\mathbf{p} = 0$; due to (g) an influence of III_p is neglected). The system (5.1) to (5.3) represents an extension of Odquist-Hoff's law [15].

Adequate information needed for the solution of the inverse problem for $\bar{d}_1$ can be obtained from a series of tensile tests. If initially identical specimens are deformed at various rates v and temperatures θ, and the force $F = \bar{F}(t, \theta, v)$ necessary to maintain the deformation is registered, we can easily get

$$p = \bar{p}(t, \theta, v), \qquad T = \bar{T}(t, \theta, v), \tag{5.4}$$

where p and T are the components of $\mathbf{p}$ and $\mathbf{T}$ in the direction of the tensile axis.

The solution of the inverse problem is then

$$\bar{d}_1(\mathrm{II}_p, \theta, \mathrm{II}) = (1/T)\frac{\partial \bar{p}}{\partial t}. \tag{5.5}$$

In $\partial\bar{p}/\partial t$ we substitute for $v = \bar{g}_1(T, \theta, p)$ and $t = \bar{g}_2(T, \theta, p)$, where $\bar{g}_1$, $\bar{g}_2$ are obtained by inversion of (5.4) with respect to t and v; further we use $T = \sqrt{-3\,\mathrm{II}}$, $p = 2\sqrt{-\mathrm{II}_p/3}$.

In the preliminary experiments a series of cylindrical mild steel specimens [2] of the gauge length 2.6cm and the diameter 0.4 cm were tested in tension on an Instron tensile testing machine at crosshead speeds 0.005cm/min, 0.2cm/min, 5cm/min, and temperatures 295°K, 335°K, 375°K in the range up to 15% elongation. Data obtained from the relation (5.5) were approximated by the formula [the analytical relation of the type (5.6) appears in the work-hardening theory [17] and is used in [18]; the details of the dependence (5.5) in the vicinity of the yield point are not adequately reproduced by (5.6)]

$$\bar{d}_1(\bar{\mathrm{II}}_p, \theta, \bar{\mathrm{II}}) = \frac{c_1}{\bar{\bar{\mathrm{II}}}} \exp\left[-\frac{c_2}{\theta}\left(1-\frac{\bar{\mathrm{II}}-\sqrt{\alpha}}{c_3}\right)^2\right] \tag{5.6}$$

[2] Mild steel delivered in rolled bars and annealed for recrystallization has standardized composition: C 0.07–0.14%, Mn 0.35–0.65%, Si 0.17–0.37%, Cr, Ni, Cu, P, S, resp. at most 0.15, 0.30, 0.04, 0.04%, resp. X-ray diffraction patterns indicated relatively large grain of the order 10^{-2}mm and no detectable preferred orientation (radiation CoKα, collimator of the diameter 1mm) [16].

as long as $\overline{\text{II}} > \sqrt{\alpha}$, and $\bar{d}_1 = 0$ if $\overline{\text{II}} \leqslant \sqrt{\alpha}$. The quantity $\alpha = |c_4 \overline{\text{II}}_p + c_5|$, and $\overline{\text{II}} = \sqrt{\operatorname{tr} \mathbf{T}^2} = \sqrt{2\text{II}}$, $\overline{\text{II}}_p = \sqrt{\operatorname{tr} \mathbf{p}^2} = \sqrt{-2\text{II}_p}$. The following values of the constants were used: $c_1 = 20.4\,\text{kp}^{-2}\text{cm}^4\text{sec}^{-1}$, $c_2 = 8.2\times 10^4\,\text{K}$, $c_3 = 2.1\times 10^3\,\text{kp}\,\text{cm}^{-2}$,

$$c_4 = 3.64\times 10^7\ \text{kp}^2\text{cm}^{-4},\ c_5 = -3.4\times 10^5\,\text{kp}^2\text{cm}^{-4}.$$

The constitutive equations (5.1) to (5.3) with determined $\bar{d}_1$ can be used to predict the behaviour of studied mild steel in thermo-mechanical processes which fall within the limits set up by the restriction (a) to (j). As an example we used the constitutive equations (5.1) to (5.3) with $\bar{d}_1$ given by (5.6) in solution of a coupled thermoplastic heat-conduction problem of torsion of a steel shaft. The specimens made of the same material as the tensile test specimens had the gauge length 14.5 cm and the diameter 1.5 cm; deformation rate was one revolution per 27.5 sec, shear modulus $8.38\times 10^5\,\text{kp}\,\text{cm}^{-2}$ [16], heat capacity $0.109\,\text{cal}\,\text{g}^{-1}\text{K}^{-1}$ [19], heat conductivity $0.17\,\text{cal}\,\text{cm}^{-1}\text{sec}^{-1}\text{K}^{-1}$ [19] and density $7.87\,\text{g}\,\text{cm}^{-3}$

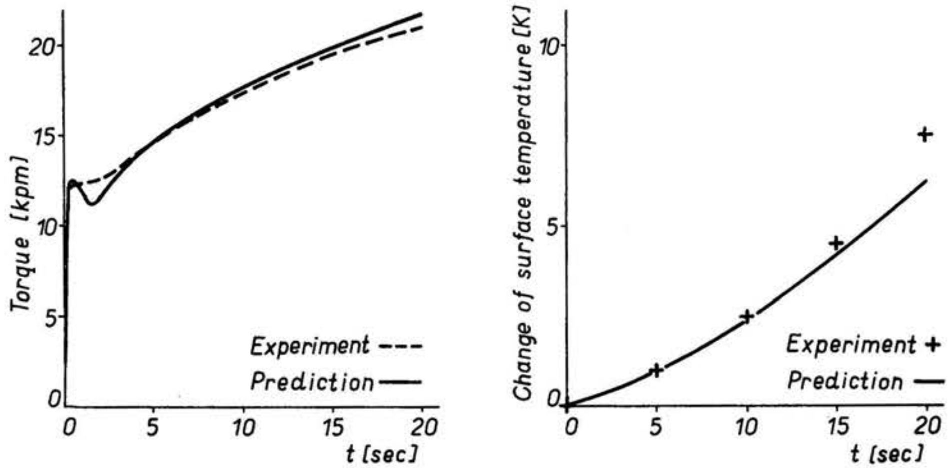

FIG. 1. Preliminary results of torsion experiments on mild steel shaft and the comparison with predicted values of torque and surface temperature.

[19]. The theoretical predictions of torque and surface temperature obtained by the method described in detail in [18] are compared with experimental values on Fig. 1 (the torsion experiments were performed on a Mohr & Federhaff torsion testing machine with a pendulum dynamometer, for temperature measurement a chromel-aluminium thermocouple was used; in theoretical calculations a thermal isolation of the surface of the specimen was assumed).

6. Conclusion

The proposed method of the determination of the concrete form of inelastic constitutive equations is divided into three steps:

(i) A sufficiently general form of constitutive equations derived in the thermodynamics of inelastic materials is specified at the outset. The internal variable approach is adopted.

(ii) Specific information on studied class of materials and thermo-mechanical processes are listed and used to restrict the generality of the constitutive equations adopted by step (i); thus, the number of unknown constitutive functions is reduced.

(iii) The inverse problem for the remaining unknown constitutive functions is formulated and solved. Within the framework of the internal variable approach to inelasticity the inverse problem is reduced to differentiation, inversion and interpolation of functions derived from suitably designed experiments. The number and complexity of the needed experiments increase rapidly with the number of remaining unknown constitutive functions and the number of their variables.

The critical point of the practical application of the proposed method is to find in step (ii) the restrictions adequate to a studied situation. The restrictions have to balance two competitive features: (1) the accuracy and the range of validity of the derived concrete form of the constitutive equations delimited by step (ii); (2) the number and complexity of measurements needed for the solution of the corresponding inverse problem.

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