Arch. Mech., 50, 2, pp. 247–263, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

A self-consistent model of rate-dependent plasticity of polycrystals

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THE HILL–HUTCHINSON self-consistent scheme for polycrystals is extended to rate-dependent plasticity with work-hardening. A computational version of the model requires three material parameters for a single crystal which are approximately identified from the experimental stress – plastic strain curve for a polycrystalline material. Contours of the macroscopic plastic potential are calculated after different plastic prestrains in uniaxial tension.

1. Introduction

IN THE CLASS of "self-consistent" models of a polycrystalline aggregate, an auxiliary problem is formulated for a single crystal (inclusion) embedded in a homogeneous medium (matrix) of some different material (HILL [1]). For path-dependent plastic materials, the typical problem is that of *incremental* equilibrium, and a deformation process is analyzed step by step. To take advantage of ESHELBY'S [2] solution, which is uniform within an ellipsoidal inclusion, the auxiliary problem must be posed as *linear*, that is, at the current step of computations all relevant parameters of the matrix material must be treated as constants. On the other hand, for adequate modeling of the interaction between a crystal and the surrounding aggregate of grains, it is proper to assign to the matrix the actual overall properties of the polycrystal. It is not evident how to reconcile both requirements when the grains undergo elastic-plastic deformation so that the overall response of the polycrystal is not incrementally linear.

In a number of papers, the matrix material in the auxiliary problem was characterized by the constants of linear elasticity. The aforementioned interaction was in effect modeled as purely elastic, irrespectively of the average plastic strain attributed to the matrix. That approach was originally developed for small-strain rate-independent plasticity (KRÖNER [3], BUDIANSKY and WU [4]) and extended to creep (BROWN [5]) and rate-dependent plasticity in the framework of small strain (WENG [6]) and of large strain (NEMAT–NASSER and OBATA [7], HARREN [8]). During advanced plastic flow, the flexibility of the constraints of a grain is most likely underestimated in that way with respect to the actual constraints within the aggregate.

That deficiency was removed in HILL'S [1] formulation who proposed to use, in the auxiliary incremental problem for rate-independent plasticity, the instantaneous compliances that connect the *actual* rates of overall stress and strain

of the polycrystal. This can be justified by appealing to the homogeneity of degree zero of the compliances, and offers the possibility to incorporate plastic anisotropy of the polycrystal to the definition of the matrix material. Since the compliances are unknown in advance, the increased accuracy of that approach is connected with a greater computational effort in comparison with the use of elastic moduli. HUTCHINSON [9] demonstrated that the approach is numerically applicable in the case of transversal isotropy at small strain. An extension to finite strain was formulated by IWAKUMA and NEMAT-NASSER [10] and applied to two-dimensional problems. The behaviour of a three-dimensional self-consistent model of a time-independent elastic-plastic polycrystal was analysed numerically by LIPIŃSKI *et al.* [11].

An intermediate approach was proposed by BERVEILLER and ZAOUI [12] who retained the formulae for an elastically isotropic matrix but with the material stiffness parameter modified, e.g. in order to correspond to the secant modulus. A similar concept was also applied to viscoplastic polycrystals (CAILLETAUD [13]).

Rate-dependent elasto-plastic polycrystals were also investigated by using the self-consistent scheme with approximately defined inelastic properties of the matrix. NEMAT-NASSER and OBATA [7] proposed the matrix moduli derived from certain local moduli dependent explicitly on the assumed time step. MOLINARI *et al.* [14] defined the moduli by linearizing around the current strain-rate the nonlinear relationship between the plastic part of strain-rate and stress. Another approach based on the adaptation of the self-consistent scheme developed for linear viscoelasticity was recently proposed by NAVIDI *et al.* [15] and illustrated by the example of an isotropic multiphase material.

HUTCHINSON [16] showed that Hill's method can be applied to examining steady creep without the need of approximating the actual nonlinear constitutive relation between the strain-rate and stress. As the basic step in the absence of elasticity effects, the linear auxiliary problem was posed in a natural way in terms of the *differentials* of strain-rate and stress, related to each other in a given state by the tensor of creep compliances independent of those differentials(1). Hutchinson's analysis was limited to steady deformations of non-hardening materials.

The aim of this paper(2) is to extend the Hill-Hutchinson self-consistent model of polycrystals to rate-dependent plasticity with work-hardening. Certain additional terms will appear in the basic equations since HILL'S [1] theory did not deal with rate-dependence effects, and HUTCHINSON'S [16] model did not account for work-hardening. To retain consistency, elastic compliances are neglected at the outset. Accordingly, the model is suited for simulation of developed plastic flow rather than of the range where the aggregate is predominantly elastic, just

(1) The restriction to a non-hardening material obeying a power crep law allowed the system of incremental equation to be integrated to a total form.

(2) Based on the former author's Ph.D. Thesis [17].

contrary to the models which use elastic compliances for defining the matrix material.

A three-parameter computational version of the model is applied here to simulate uniaxial tension of an aluminum alloy. An approximate procedure is proposed for identifying the material parameters for a single crystal from the standard uniaxial tension test of a polycrystalline specimen. The calculated stress-strain curve and contours of a visco-plastic potential at various stages of the deformation serve as examples of the predictions of the model. A comparison is made with the experimental stress-strain curve and conventional yield surfaces.

Throughout this paper any changes in geometry during deformation are disregarded, i.e. the small strain formulation is used and lattice rotations are neglected. Bold-face small letters, Roman or Greek, denote second-order symmetric tensors, and bold-face capital letters denote fourth-order tensors possessing the minor symmetries, with the respective unit tensor denoted by $\mathbf{I}$ and the transpose indicated by a superscript T. A juxtaposition of two tensor symbols denotes double contraction. A superimposed dot over a symbol denotes the material time derivative, understood as a forward rate.

2. General equations of the model

2.1. Constitutive framework of rate-dependent plasticity

Constitutive equations of isothermal rate-dependent plasticity are assumed in the following general form

$$\begin{aligned} \dot{\boldsymbol{\varepsilon}} &= \dot{\boldsymbol{\varepsilon}}^p + \dot{\boldsymbol{\varepsilon}}^e, \qquad & \dot{\boldsymbol{\varepsilon}}^e &= \mathbf{M}^e\, \dot{\boldsymbol{\sigma}}, \\ \dot{\boldsymbol{\varepsilon}}^p &= \mathbf{f}(\boldsymbol{\sigma}, g_K), \qquad & \dot{g}_K &= \mathrm{g}_K(\boldsymbol{\sigma}, g_L), \end{aligned} \tag{2.1}$$

where $\mathbf{f}$ and g_K are sufficiently smooth, given functions. In the small strain formulation adopted, $\dot{\boldsymbol{\varepsilon}}^e$ and $\dot{\boldsymbol{\varepsilon}}^p$ are the elastic and plastic parts, respectively, of the small-strain rate, and $\dot{\boldsymbol{\sigma}}$ is the rate of the Cauchy stress. The elastic strain-rate $\dot{\boldsymbol{\varepsilon}}^e$ is related to $\dot{\boldsymbol{\sigma}}$ by the fourth-order tensor $\mathbf{M}^e$ of elastic compliances, while $\dot{\boldsymbol{\varepsilon}}^p$ is a function of the current material state, represented here by the stress $\boldsymbol{\sigma}$ and a certain number P of material parameters g_K $(K = 1, ..., P)$. The latter need not be interpreted as internal state variables, and for anisotropic materials they can be regarded as either scalars or components of tensor variables for a fixed orientation of a material element relative to a given reference frame. In the computational version of the model and at the level of a single crystal, g_K will be identified with the current critical resolved shear stress on the K-th slip system.

Elasticity effects during plastic flow will be neglected, so that we will substitute

$$\mathbf{M}^e \cong \mathbf{0}, \qquad \dot{\boldsymbol{\varepsilon}} \cong \dot{\boldsymbol{\varepsilon}}^p, \tag{2.2}$$

but *conceptually* the elastic compliances will be treated as vanishingly small rather than as being exactly zero. The distinction will become important in the presence of discontinuous changes in stress, in particular in the calculations of an instantaneous overall plastic potential.

Assuming that $\mathbf{f}$ is differentiable with respect to its arguments, we can write

$$\ddot{\boldsymbol{\varepsilon}} = \mathbf{M}\,\dot{\boldsymbol{\sigma}} + \ddot{\boldsymbol{\varepsilon}}^r, \tag{2.3}$$

where $\mathbf{M}$ and $\ddot{\boldsymbol{\varepsilon}}^r$ are functions only of the material state, viz.

$$\mathbf{M} = \mathbf{M}(\boldsymbol{\sigma}, g_K) \equiv \mathbf{f}_{,\boldsymbol{\sigma}}(\boldsymbol{\sigma}, g_K), \qquad \ddot{\boldsymbol{\varepsilon}}^r \equiv \sum_K \mathbf{f}_{,g_K}(\boldsymbol{\sigma}, g_J)\mathrm{g}_K(\boldsymbol{\sigma}, g_L); \tag{2.4}$$

a comma followed by an index denotes partial differentiation. It follows that in a given state of the material, the *second* rate of strain is a *linear*, although inhomogeneous, function of stress-rate. At the moment we do not assume that a plastic potential exists so that $\mathbf{M}$ need not be symmetric in general.

Under the assumption (2.2) of negligible elastic compliances, the relationship (2.3) characterizes a rate-dependent plastic response at either level of constitutive description. By using a subscript c for constitutive quantities at the level of a single crystal (grain), we shall write

$$\ddot{\boldsymbol{\varepsilon}}_c = \mathbf{M}_c\,\dot{\boldsymbol{\sigma}}_c + \ddot{\boldsymbol{\varepsilon}}_c^r. \tag{2.5}$$

Overall (macroscopic) quantities will be distinguished by a superimposed bar, while unweighted volume averaging will be denoted by curly brackets. By defining the overall stress $\overline{\boldsymbol{\sigma}}$ and strain $\overline{\boldsymbol{\varepsilon}}$ as

$$\overline{\boldsymbol{\sigma}} = \{\boldsymbol{\sigma}_c\}, \qquad \overline{\boldsymbol{\varepsilon}} = \{\boldsymbol{\varepsilon}_c\}, \tag{2.6}$$

the constitutive relationship (2.3) for a polycrystal reads

$$\ddot{\overline{\boldsymbol{\varepsilon}}} = \mathbf{M}\,\dot{\overline{\boldsymbol{\sigma}}} + \ddot{\overline{\boldsymbol{\varepsilon}}}^r. \tag{2.7}$$

Our primary task is now to express $\mathbf{M}$ and $\ddot{\overline{\boldsymbol{\varepsilon}}}^r$ in terms of $\mathbf{M}_c$ and $\ddot{\boldsymbol{\varepsilon}}_c^r$.

2.2. Self-consistent method

Following HILL [1], consider the auxiliary incremental problem for an ellipsoidal inclusion embedded in an infinite homogeneous matrix. The inclusion represents a single grain and the matrix replaces the polycrystalline material surrounding the grain. A uniform stress $\boldsymbol{\sigma}_c$ within each grain and the average stress in the matrix, taken equal to $\overline{\boldsymbol{\sigma}}$ by assumption, are regarded as known, along with the current values of all material parameters. Then, in contrast to Hill's work concerned with rate-independent plasticity, the (plastic) strain rate $\dot{\boldsymbol{\varepsilon}}_c^p = \dot{\boldsymbol{\varepsilon}}_c$ in

each grain (and also the average strain rate $\dot{\bar{\boldsymbol{\varepsilon}}}$) are also known from the constitutive equations of rate-dependent plasticity at the micro-level. The auxiliary problem is posed here in terms of the differentials $d\boldsymbol{\sigma}_c$, $d\dot{\boldsymbol{\varepsilon}}$ and $d\bar{\boldsymbol{\sigma}}$, $d\dot{\bar{\boldsymbol{\varepsilon}}}$, or equivalently, in terms of stress-rates $\dot{\boldsymbol{\sigma}}_c$, $\dot{\bar{\boldsymbol{\sigma}}}$ and of the *second-order* rates of strain, $\ddot{\boldsymbol{\varepsilon}}$, $\ddot{\bar{\boldsymbol{\varepsilon}}}$. From (2.5) and (2.7) it follows that the problem is *linear* but inhomogeneous; an analogous problem but without the additive non-homogeneous term was examined by HUTCHINSON [16]. Here, $d\bar{\boldsymbol{\sigma}} = \mathbf{0}$ does not imply $d\boldsymbol{\sigma}_c = \mathbf{0}$ so that stress redistribution in the polycrystal takes place also at a constant overall stress. The Hill–Hutchinson self-consistent scheme has thus to be modified([3]).

For this purpose, we observe first that the relationship between a *difference* $\Delta\dot{\boldsymbol{\sigma}}$ in two uniform fields of stress-rate within an ellipsoidal hole in the matrix and a difference $\Delta\ddot{\boldsymbol{\varepsilon}}$ in the associated second-order rates of straining of the ellipsoid is still linear homogeneous,

$$\Delta\ddot{\boldsymbol{\varepsilon}} = -\mathbf{M}^*\Delta\dot{\boldsymbol{\sigma}}, \tag{2.8}$$

where $\mathbf{M}^*$ can be connected with the Eshelby tensor $\mathbf{S}$ [2] for the matrix with a constant compliance tensor $\mathbf{M}$ by the equation [1]

$$(\mathbf{I} - \mathbf{S})\mathbf{M}^* = \mathbf{S}\,\mathbf{M}. \tag{2.9}$$

It should be noted that in the derivation of (2.8), the matrix is treated as being in a uniform stress state at the instant under consideration, which is an additional assumption [16].

By identifying $\Delta\dot{\boldsymbol{\sigma}}$ with $\dot{\boldsymbol{\sigma}}_c - \dot{\bar{\boldsymbol{\sigma}}}$ and $\Delta\ddot{\boldsymbol{\varepsilon}}$ with $\ddot{\boldsymbol{\varepsilon}}_c - \ddot{\bar{\boldsymbol{\varepsilon}}}$, and substituting (2.5) and (2.7), from (2.8) we obtain

$$(\mathbf{M}^* + \mathbf{M}_c)\dot{\boldsymbol{\sigma}}_c = (\mathbf{M}^* + \mathbf{M})\dot{\bar{\boldsymbol{\sigma}}} - \left(\ddot{\boldsymbol{\varepsilon}}_c^r - \ddot{\bar{\boldsymbol{\varepsilon}}}^r\right). \tag{2.10}$$

This relationship differs from an analogous equation given by HILL [1] merely by the last additive term which is independent of the overall stress-rate. We may thus define the "concentration-factor tensor" $\mathbf{B}_c$ by the unchanged formula([4])

$$\mathbf{B}_c = (\mathbf{M}^* + \mathbf{M}_c)^{-1}(\mathbf{M}^* + \mathbf{M}). \tag{2.11}$$

By introducing the following expression for a relaxation stress-rate

$$\dot{\boldsymbol{\sigma}}_c^r = -(\mathbf{M}^* + \mathbf{M}_c)^{-1}\left(\ddot{\boldsymbol{\varepsilon}}_c^r - \ddot{\bar{\boldsymbol{\varepsilon}}}^r\right), \tag{2.12}$$

we arrive at

$$\dot{\boldsymbol{\sigma}}_c = \mathbf{B}_c\dot{\bar{\boldsymbol{\sigma}}} + \dot{\boldsymbol{\sigma}}_c^r. \tag{2.13}$$

([3]) Similar modification was done in earlier papers in the context different from the present one, without appealing to the second-order rate of strain.

([4]) All matrices are implicity assumed to be invertible if needed.

Note that $\mathbf{B}_c$ and $\dot{\boldsymbol{\sigma}}_c^r$ are uniquely defined in the current state, independently of the overall stress-rate.

By substituting (2.13) into (2.5), we obtain

$$\ddot{\boldsymbol{\varepsilon}}_c = \mathbf{M}_c \mathbf{B}_c \dot{\bar{\boldsymbol{\sigma}}} + \mathbf{M}_c \dot{\boldsymbol{\sigma}}_c^r + \ddot{\boldsymbol{\varepsilon}}_c^r . \tag{2.14}$$

Now, by taking the volume averages of (2.13), (2.14) and comparing with (2.6), we obtain the known pair of self-consistency conditions

$$\{\mathbf{B}_c\} = \mathbf{I}, \qquad \{\mathbf{M}_c \mathbf{B}_c\} = \mathbf{M} \tag{2.15}$$

along with another pair

$$\{\dot{\boldsymbol{\sigma}}_c^r\} = \mathbf{0}, \qquad \{\mathbf{M}_c \dot{\boldsymbol{\sigma}}_c^r + \ddot{\boldsymbol{\varepsilon}}_c^r\} = \ddot{\bar{\boldsymbol{\varepsilon}}}^r. \tag{2.16}$$

For spherical grains when $\mathbf{M}^*$ depends only on $\mathbf{M}$, the conditions in (2.16) are equivalent to each other, as can be seen by taking the average of both sides of (2.12) multiplied beforehand by $(\mathbf{M}^* + \mathbf{M}_c)$.

The conditions (2.15) and (2.16) can further be transformed to a form which will appear more convenient in calculations. From (2.15) we immediately obtain

$$\{(\mathbf{M} - \mathbf{M}_c)\mathbf{B}_c\} = \mathbf{0}, \tag{2.17}$$

with an advantage that the averaged expression possesses diagonal symmetry if $\mathbf{M}_c$ and $\mathbf{M}$ do [16]. For spherical grains, or for $\mathbf{M}^*$ dependent only on $\mathbf{M}$, the condition $(2.16)_1$ rearranged with the help of (2.12), (2.11) and $(2.15)_1$ yields

$$\ddot{\bar{\boldsymbol{\varepsilon}}}^r = \{\ddot{\boldsymbol{\varepsilon}}_c^r \widehat{\mathbf{B}}_c\}, \qquad \widehat{\mathbf{B}}_c = \left(\mathbf{M}^{*T} + \mathbf{M}_c^T\right)^{-1} \left(\mathbf{M}^{*T} + \mathbf{M}^T\right), \tag{2.18}$$

where $\widehat{\mathbf{B}}_c$ reduces to $\mathbf{B}_c$ if $\mathbf{M}_c$ and $\mathbf{M}$ possess diagonal symmetry.

2.3. Plastic potential

Suppose now that the relationship between $\dot{\boldsymbol{\varepsilon}}_c^p$ and $\boldsymbol{\sigma}_c$ admits a potential, viz.

$$\dot{\boldsymbol{\varepsilon}}_c^p = \frac{\partial \omega_c(\boldsymbol{\sigma}_c, g_K)}{\partial \boldsymbol{\sigma}_c} . \tag{2.19}$$

For instance, let $\dot{\boldsymbol{\varepsilon}}^p$ in a given grain be a sum of the strain rates due to slipping on N individual slip systems defined by the two unit vectors: the slip direction $\mathbf{m}^K$ and the normal $\mathbf{n}^K$ to the slip plane, so that

$$\dot{\boldsymbol{\varepsilon}}_c^p = \sum_K \dot{\gamma}^K \boldsymbol{\alpha}^K, \qquad \boldsymbol{\alpha}^K = \frac{1}{2}\left(\mathbf{m}^K \otimes \mathbf{n}^K + \mathbf{n}^K \otimes \mathbf{m}^K\right), \qquad K = 1, ..., N, \tag{2.20}$$

where $\dot{\gamma}^K$ is a slip rate on the K-th system. If any $\dot{\gamma}^K$ depends on $\boldsymbol{\sigma}_c$ only through the shear stress resolved on the K-th slip system, that is, if

$$\dot{\gamma}^K = \dot{\gamma}^K(\tau^K, g_L), \qquad \tau^K = \boldsymbol{\sigma}_c \boldsymbol{\alpha}^K \tag{2.21}$$

then (2.19) is satisfied (Kestin and Rice [18]); this can be verified by substituting

$$\omega_c(\boldsymbol{\sigma}_c, g_L) = \int_0^{\boldsymbol{\sigma}_c} \mathbf{f}(\boldsymbol{\sigma}, g_L)\, d\boldsymbol{\sigma} = \sum_K \int_0^{\tau^K} \dot{\gamma}^K(\tau, g_L)\, d\tau. \tag{2.22}$$

If (2.19) holds then $\mathbf{M}_c = \partial^2 \omega_c / \partial \boldsymbol{\sigma}_c \partial \boldsymbol{\sigma}_c$ is diagonally symmetric. Then, we can conclude (cf. HILL [19], HILL and RICE [20]) about diagonal symmetry of $\mathbf{M}$ from the assumed equality of work differentials at the micro and macro-levels expressed in the *incremental* form as

$$\dot{\bar{\boldsymbol{\varepsilon}}}\, \delta\bar{\boldsymbol{\sigma}} = \{\dot{\boldsymbol{\varepsilon}}\, \delta\boldsymbol{\sigma}\}, \tag{2.23}$$

where $\delta\boldsymbol{\sigma}$ is a statically admissible field of a stress increment such that $\{\delta\boldsymbol{\sigma}\} = \delta\bar{\boldsymbol{\sigma}}$, which need not be related to a (compatible) field $\dot{\boldsymbol{\varepsilon}}$. In particular, (2.23) holds if the prefix δ refers to a purely *elastic* change of the stress field within the aggregate; this is not in contradiction with our assumption that elastic compliances are negligibly small (but *not* exactly zero) since the proportional scaling down of elastic compliances does not influence the distribution of $\delta\boldsymbol{\sigma}$ obtained for given $\delta\bar{\boldsymbol{\sigma}}$. Following RICE [21], or simply by substituting (2.2) and (2.19) into the equality (2.23), the constitutive relationship for a polycrystal can be expressed in terms of a macroscopic potential Ω, viz.

$$\Omega = \{\omega_c\}, \qquad \dot{\bar{\boldsymbol{\varepsilon}}}^p = \frac{\partial \Omega}{\partial \bar{\boldsymbol{\sigma}}}, \qquad \mathbf{M} = \frac{\partial^2 \Omega}{\partial \bar{\boldsymbol{\sigma}}\, \partial \bar{\boldsymbol{\sigma}}}. \tag{2.24}$$

3. Three-parameter version of the model

For computational purposes we assume the constitutive equations for $\dot{\boldsymbol{\varepsilon}}^p$ in the form (2.20) and, following many other authors (e.g. BROWN [5], PAN and RICE [22], ASARO and NEEDLEMAN [23]), specify the rate-dependence expression $(2.21)_1$ as a power law

$$\dot{\gamma}_K = \dot{\gamma}^0 \left| \frac{\tau_K}{g_K} \right|^{1/m} \operatorname{sgn}(\tau_K) \tag{3.1}$$

with $K = 1, \ldots, 12$ ($P = N = 12$) and $\boldsymbol{\alpha}_K$ corresponding to fundamental slip systems in fcc crystals. $\dot{\gamma}^0$ is not an independent material parameter but plays the role of a given time-scale factor. Evolution equations for the parameters g_K

(for $0 < m \ll 1$ interpreted as critical values of the resolved shear stress) are assumed in the usual rate form

$$g_K = \sum_L h_{KL} |\dot{\gamma}_L| . \tag{3.2}$$

In the simplest version of the model, we will assume linear hardening obeying the Taylor hypothesis, $h_{KL} = h = \text{const}$. As the initial condition for (3.2) in a virgin state of a macroscopically isotropic polycrystal we take $g_K = \tau^0$, where τ^0 is the initial critical value for τ_K, the same for all slip systems.

The expression (2.22) for the local plastic potential reduces to

$$\omega_c = \frac{m}{1+m} \sum_K \tau_K \dot{\gamma}_K = \frac{m}{1+m} \boldsymbol{\sigma}_c \dot{\boldsymbol{\varepsilon}}_c^p . \tag{3.3}$$

To calculate the macroscopic plastic potential Ω, we need a relationship between purely elastic stress increments at the micro and macro-levels. The simplest assumption is to neglect elastic heterogeneity (and thus *elastic* anisotropy of crystals), which means that $\delta\boldsymbol{\sigma} \equiv \delta\overline{\boldsymbol{\sigma}}$. Then, at a fixed distribution of g_K within the aggregate, we obtain

$$\Omega(\overline{\boldsymbol{\sigma}} + \Delta\overline{\boldsymbol{\sigma}}) = \frac{m}{1+m} \left\{ (\boldsymbol{\sigma}_c + \Delta\overline{\boldsymbol{\sigma}}) \dot{\boldsymbol{\varepsilon}}_c^p (\boldsymbol{\sigma}_c + \Delta\overline{\boldsymbol{\sigma}}) \right\}, \tag{3.4}$$

where $\overline{\boldsymbol{\sigma}}$ and $\boldsymbol{\sigma}_c$ are the current macro and micro-stresses, respectively, and $\Delta\overline{\boldsymbol{\sigma}}$ stands for an instantaneously applied finite increment of the macroscopic stress, corresponding to purely elastic response of the aggregate.

To summarize, in the simplest computational version of the proposed model there are three independent material parameters assumed at the micro-level: m, τ^0 and h. In the next section, an approximate procedure is proposed for the identification of these parameters from the standard uniaxial tension test performed on a *polycrystalline* specimen.

The numerical implementation of the self-consistent scheme (more details are given in [17]) has followed closely that described by HUTCHINSON [16] and employed the (corrected) formulae given by KNEER [24] for a spherical inclusion in a transversally isotropic matrix. Volume averaging in the simulation of uniaxial tension was replaced by the averaging over 36 orientations of fcc crystals corresponding to different values of *two* Euler angles. In the calculations of the plastic potential, this has been complemented by additional averaging over 12 values of the third Euler angle that defines rotation about the tensile axis.

4. An approximate identification procedure

Suppose that the stress – plastic strain curve obtained experimentally from the standard uniaxial tension test, within some strain interval of developed

plastic flow, can be approximated by a linear segment whose slope defines the macroscopic hardening modulus, say H. A sample result of that type is presented in Fig. 1 which has been obtained for an aluminum alloy PA6 at the room temperature([5]). To eliminate the influence of an initial period of a constrained plastic flow in the grains, the macroscopic initial yield stress, say Σ^0, is defined by backward extrapolation of the linear segment up to the zero plastic strain offset. By performing at least two experiments at a different rate of stress or of plastic strain, in the standard manner we can determine the exponent $\overline{m}$ of strain-rate sensitivity of the polycrystalline material.

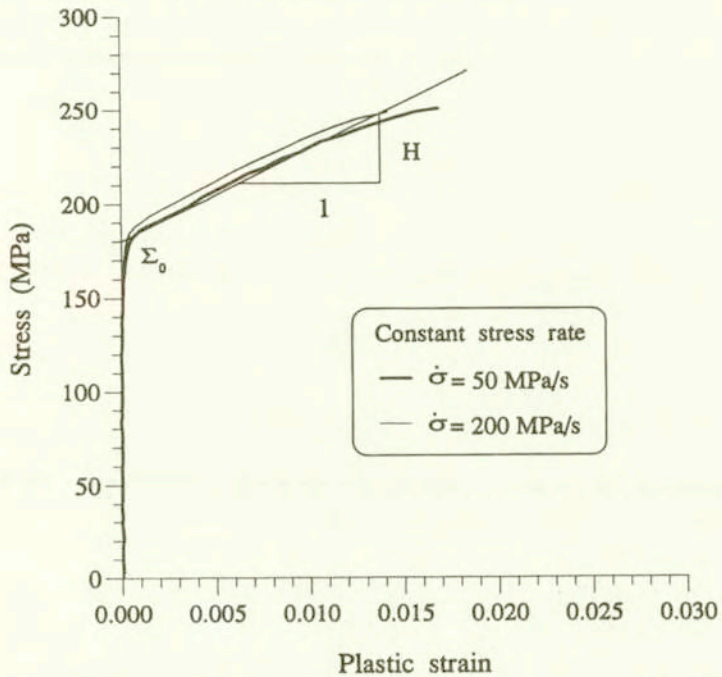


FIG. 1. Linear approximation of an initial segment of the uniaxial stress – plastic strain curve for an aluminum alloy PA6.

In that way, an approximation of the experimental relationship between the stress and plastic strain-rate in uniaxial tension of a polycrystalline specimen in a certain range of strain is constructed as

$$\dot{\overline{\varepsilon}}^p = \dot{\overline{\varepsilon}}^0 \left(\frac{\overline{\sigma}}{\Sigma^0 + H\overline{\varepsilon}^p} \right)^{1/\overline{m}} . \tag{4.1}$$

The reference strain-rate $\dot{\overline{\varepsilon}}^0$ is identified with the plastic strain rate corresponding to stress-strain curve from which the parameters Σ^0 and H have been determined.

([5]) All experimental data presented below are taken from the Thesis [17].

We proceed now to identification of the material parameters at the micro-level. The comparison of Eqs. (4.1) and (3.1) shows that a natural assumption is to take $\overline{m}$ as the rate sensitivity exponent also for a single crystal,

$$m \cong \overline{m}. \tag{4.2}$$

For many metallic materials in the room temperature, the value of the rate sensitivity parameter m is much smaller than unity. If $m \ll 1$ and if the hardening is neglected then the macroscopic stress in the range of steady viscoplastic flow under uniaxial tension is slightly smaller than τ^0 multiplied by the Taylor factor 3.06 (HUTCHINSON [16]). A similar value of that factor was found in the course of present computations, including hardening. Guided by these results, we may assume that

$$\tau^0 \cong \frac{1}{3}\Sigma^0 \tag{4.3}$$

as an approximate value of the initial yield stress for a single crystal.

From HILL'S lemma [19] applied to the uniaxial tension with elastic heterogeneity neglected, we have

$$\overline{\sigma}\,\dot{\overline{\varepsilon}}^p = \{\boldsymbol{\sigma}\,\dot{\boldsymbol{\varepsilon}}^p\} = \left\{\sum_K \tau_K \dot{\gamma}_K\right\}. \tag{4.4}$$

At small strains with $\overline{\sigma} \cong \Sigma^0$ and $\tau_K \dot{\gamma}_K \cong \tau^0 |\dot{\gamma}_K|$ for $m \ll 1$, from (4.4) and (4.3) we obtain

$$\dot{\overline{\varepsilon}}^p \cong \frac{1}{3}\left\{\sum_K |\dot{\gamma}_K|\right\}. \tag{4.5}$$

Let, as mentioned above, $\dot{\overline{\varepsilon}}^p$ be taken as the reference strain-rate $\dot{\overline{\varepsilon}}^0$, and define $\dot{\gamma}^0$ as the *mean* value of $|\dot{\gamma}_K|$. Since the number of slip systems $N = 12$, (4.5) then gives

$$\dot{\gamma}^0 \cong \frac{1}{4}\dot{\overline{\varepsilon}}^0. \tag{4.6}$$

In turn, on multiplying both sides of (4.5) by h and using the Taylor hypothesis, we obtain

$$h\dot{\overline{\varepsilon}}^p \cong \frac{1}{3}\{\dot{g}_K\} \tag{4.7}$$

for any K. Now, on the basis of (4.3) and of numerical tests, the *mean* rate $\{\dot{g}_K\}$ of the critical shear stress in the range of stabilized plastic flow at $m \ll 1$ is

postulated to be close to the macroscopic uniaxial stress-rate divided by 3. With H as the macroscopic hardening modulus, from (4.7) we finally arrive at

$$h \cong \frac{1}{9} H. \tag{4.8}$$

The material parameters m, τ_0 and h at the micro-level may can be estimated from the simple formulae (4.2), (4.3) and (4.8) if the uniaxial macroscopic law (4.1) has been given, with the relationship (4.6) between the respective time-scale factors. The identification formulae might also be applied, as they stand, to a nonlinear hardening law. A satisfactory agreement is shown below between the experimental macroscopic curve and that calculated by using the self-consistent model with the material parameters for a single crystal estimated as above. However, the applicability of the proposed identification procedure remains yet to be verified by other examples.

5. Example

In Fig. 2 the comparison is made between experimental stress – plastic strain curves for uniaxial tension of a polycrystalline aluminum alloy PA6 and those calculated numerically by using the micromechanical model described in Sec. 2. The constitutive equations have been implemented in the version specified in Sec. 3, and the material parameters have been determined according to the identification procedure described in Sec. 4. The parameter values are listed in the figure, with $n = 1/m$([6]). It can be seen that the model predicts in a satisfactory manner the character of the macroscopic stress-strain curve up to $\sim 1.5\%$ of the plastic strain. This is not just an effect of curve-fitting since the three material parameters for a single crystal have been determined beforehand and in an indirect manner. For larger strains the assumption of linear hardening has turned out to be an oversimplification and should be replaced by a nonlinear law.

Figure 3 shows the evolution of the plastic potential during the uniaxial tension of the polycrystal model in x_3-direction. The subsequent pictures correspond to the initial state and to the plastic prestrain 5% and 7%. Characteristic shape changes of the potential contours are observed: while the initial contours are ellipsoidal, subsequent contours have a rounded-off nose in vicinity of the (tensile) loading point([7]) and are flattened on the opposite (compressive) side. Simultaneously, a translation of the contours of the plastic potential towards the loading point can be observed, accompanied first by lateral contraction and then by expansion. The qualitative changes closely resemble those observed in

([6]) h_1/h_2 denotes the ratio of the diagonal to off-diagonal components of the hardening matrix for a single crystal, equal to 1 by the Taylor hypothesis.

([7]) The sharp corners that appear in the figures are due to the adopted way of graphical presentation where calculated points have been connected by straight lines.

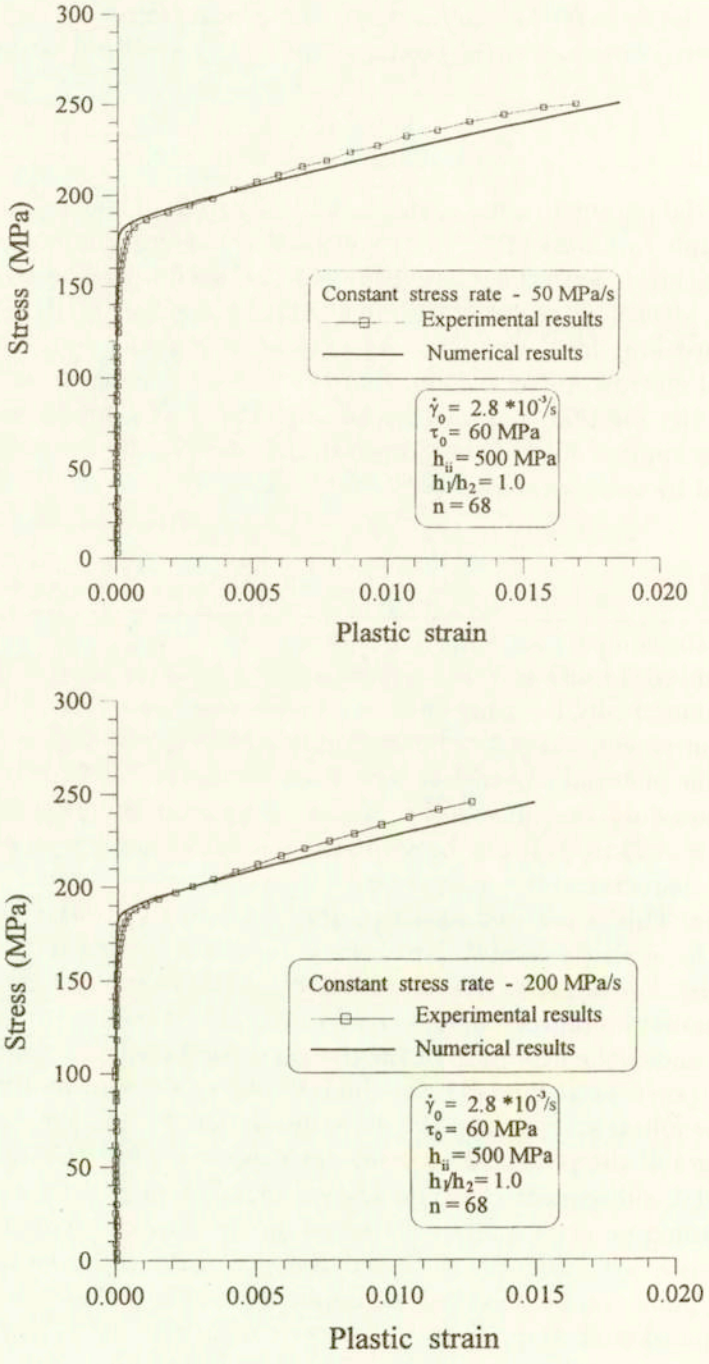
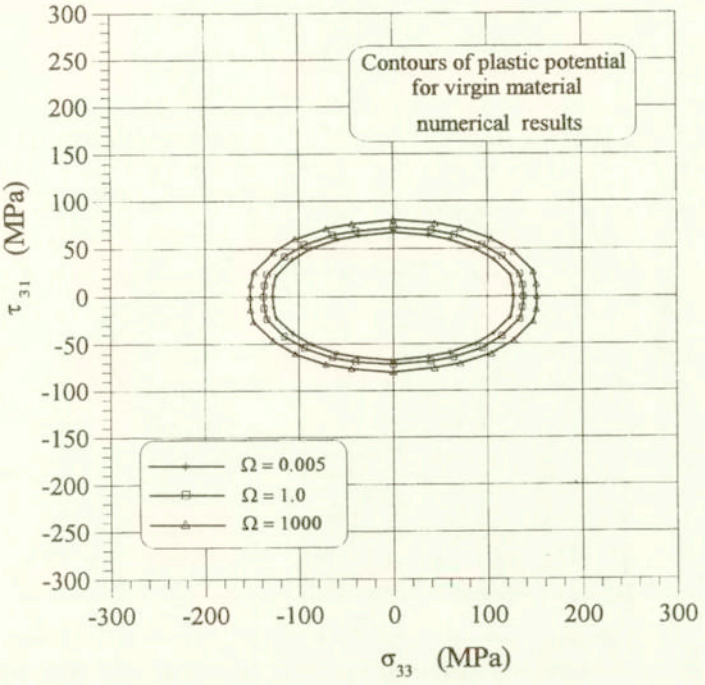
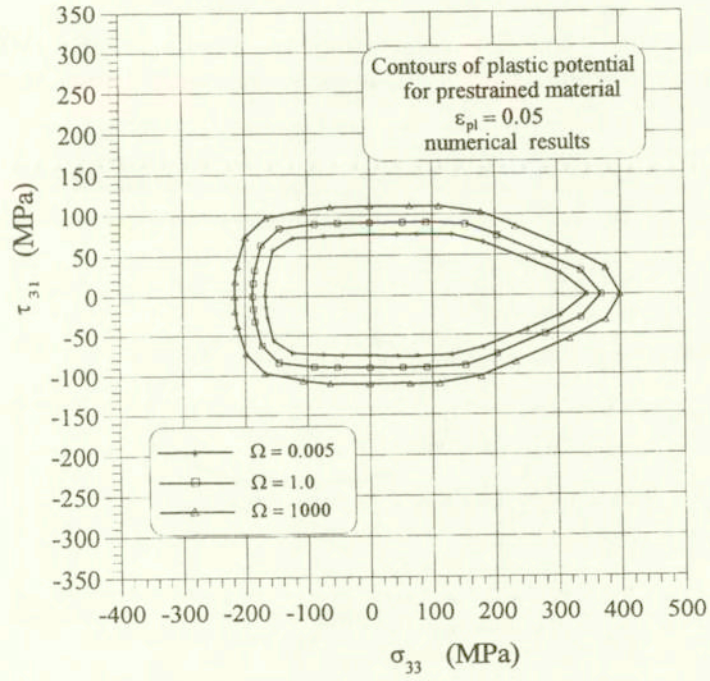


FIG. 2. Comparison of the calculated and experimental uniaxial stress – plastic strain curves at two prescribed macroscopic stress rates.





[FIG. 3 a, b]

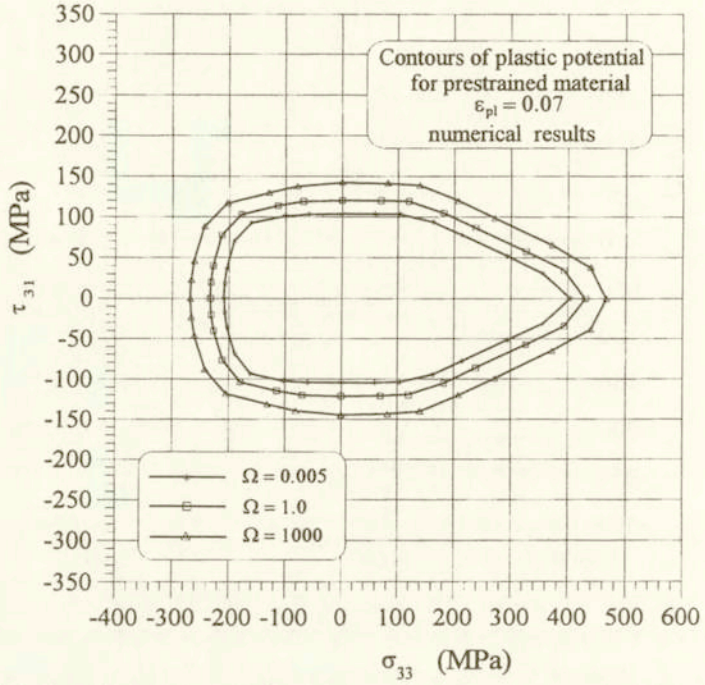
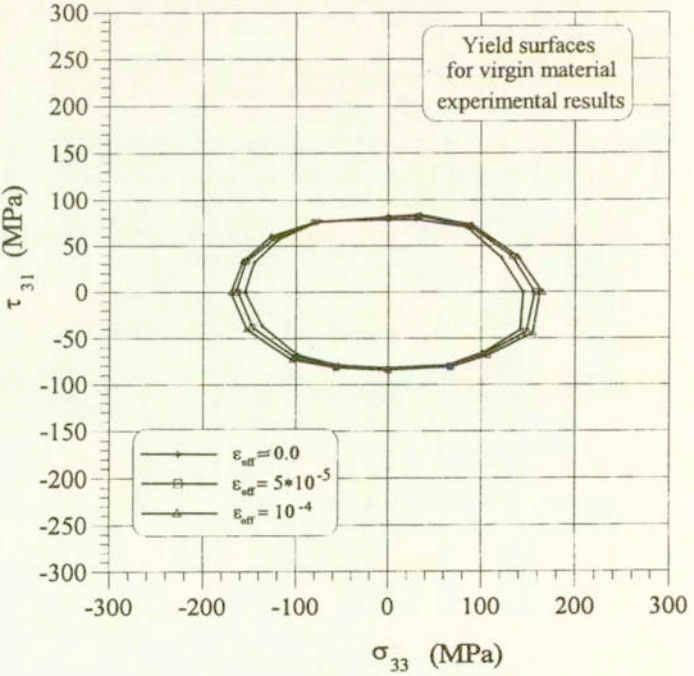
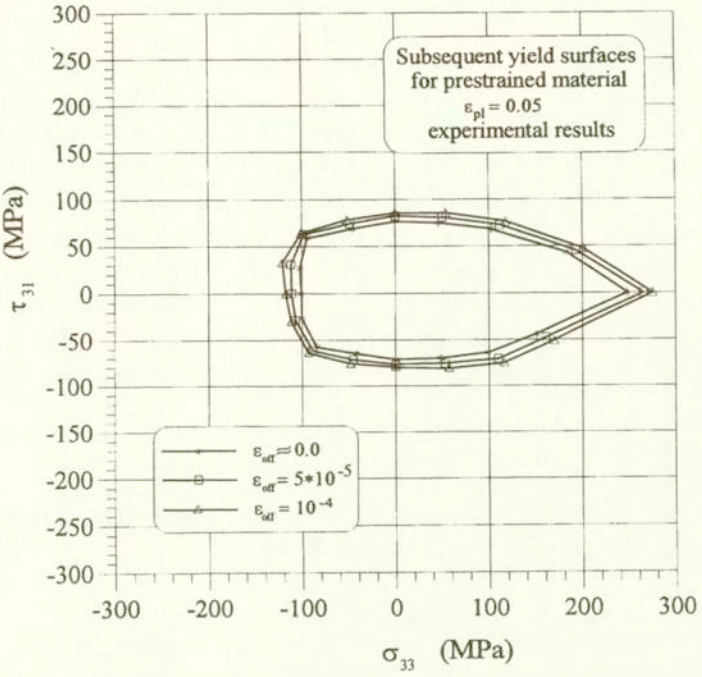


FIG. 3. Calculated contours of the macroscopic plastic potential (MPA/s) for a polycrystalline material after plastic prestrain in uniaxial tension in x_3-direction.



[FIG. 4 a]



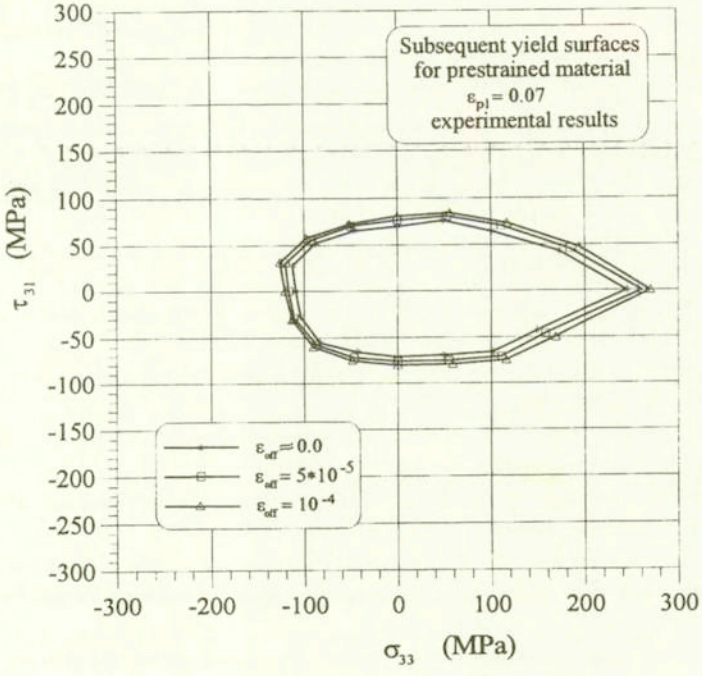


FIG. 4. Experimental yield surfaces for an aluminum alloy PA6 for various definitions of the yield offset after plastic prestrain in uniaxial tension in x_3-direction.

experimental yield surfaces for a small yield offset for the polycrystalline alloy tested, as shown in Fig. 4. This is not surprising since the contours of the plastic potential in the layer in the stress space where the potential starts to grow very rapidly, can be identified with a conventional yield surface (RICE [21]). The qualitative agreement between the calculated contours of the plastic potential for the micromechanical model shown in Fig. 3, and the respective experimental yield surfaces shown in Fig. 4, is perhaps unexpectedly good in view of the small number of material parameters in the model. This indicates that the assumptions used are likely to reflect, to a reasonable extent, the nature of plastic deformation of a polycrystalline metal under the selected monotonic loading.

Acknowledgment

This work was partially supported by the State Committee of Research (KBN) in Poland under the project No. 3 P404 035 07.

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Received December 5, 1997.