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PHENOMENOLOGICAL AND COMPUTER MODELS OF POLYCRYSTALLINE MATERIAL INELASTIC DEFORMATION

A.N. Suprun*, T.M. Vezhelis

Nizhny Novgorod State University of Architecture and Civil Engineering,

Iljinskaya St. 65, Nizhny Novgorod, 603109, Russia

*e-mail: suprun@nngasu.ru

Abstract. Variants of development of the previously obtained results aimed at increasing reliability of description of the subsequent yield surface (SYS) evolution of polycrystalline materials with the help of phenomenological models of the theory of rheonomous plasticity are suggested and briefly substantiated. The results of successful computer simulation of well-known experiments containing discrepant data on SYS are presented. The introduced phenomenological model permitted to explain the known effect of the influence of the type of unloading on an experimental SYS.

1. Introduction

It is a well-known fact that selecting phenomenological models quite adequately simulating operation of construction materials under the given physical-mechanical and other conditions today is still far from being simple. It refers to the most studied polycrystalline materials as well as widely used theories of plasticity based on the concept of subsequent yield surface of metals.

This paper is dedicated to the justification of a previously offered approach to the construction of a phenomenological model of rheonomous plasticity that comes with an agreement with modern ideas about physical processes in polycrystalline materials accompanying inelastic deformation.

2. Problems of studying subsequent yield surface in experimental mechanics

It is known (see [1, 2] and other), that until the middle of the XX century there had been no general idea about the SYS geometric form. One of the reasons for that was the fact that different traits of yield boundary in the form of angles and concavities were observed in some experiments. It should be noted, that when experimenters excluded the preload finite point from the subsequent yield surface attributes, but instead applied a sample relaxation procedure before probing, it looked like they managed to get rid of the above mentioned features of the yield boundary. But angles and concavities appeared again in experiments [3] though those rules being observed. This result was discussed in detail in [4], where the only deviation from the established methods of carrying out experiments with the subsequent yield surface was a slightly increased strain offset definition of yield. In [5] another reason was mentioned as decisive – the influence of a well-known effect of workhardening relaxation.

Still the reasons of basic differences of experimental subsequent yield surfaces constructed after partial and complete unloading of samples (see, for example, the results of experiments in [6]) have not been found. It was mentioned in [7] that those facts had not been yet explained (for more than 20 years!). At the same time it is well known that the process of

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plastic straining of polycrystalline materials is accompanied by a continuous change of the density of acquired structural defects. This density is defined by a balance between defects accumulation (that leads to the medium hardening) and their partial disappearance. Elimination of defects that takes place even after partial or complete unloading arises from the instability of the acquired faulted structure, the system's tending to the minimal internal energy, and is a natural continuation of the processes caused by material inelastic deformation. In macro-experiments this process is observed as a manifestation of a well-known effect of workhardening relaxation, that is a natural phenomenon inherent to polycrystalline materials.

Thus, it may be stated that further development of the methods of experimental study of the subsequent yield surface should be in the direction of creating mathematic and physical means of investigation of the yield surface evolution within the time interval of manifestation of the workhardening relaxation effect, as well as strain aging effect. In this case, instruments of a well-known theory of rheonomous plasticity may be used as a mathematic model that takes into account the above mentioned effects.

3. Rheonomous plasticity model

Construction of the theory of rheonomous plasticity of metals (see [8-10] and other) was carried out in the direction of the development of the associated flow law by using a hyperelliptic subsequent yield surface in the space of stresses and integral operators of the theory of viscoelasticity that derived the history of medium inelastic deformation into hyperelliptic subsequent yield surface parameters. The system of constitutive relations is oriented to plastically uncompressed and initially isotropic materials and is based on the yield surface S^* in the form of a hyperellipsoid of revolution [11] of all stress deviators $\boldsymbol{s}$ in the Euclidean space:

$$f \equiv \frac{1}{b^2}(\boldsymbol{s}-\boldsymbol{r})\cdot(\boldsymbol{s}-\boldsymbol{r})+\left(\frac{1}{a^2}-\frac{1}{b^2}\right)\left[(\boldsymbol{s}-\boldsymbol{r})\cdot\boldsymbol{\mu}\right]^2-1=0, \tag{1}$$

where a is the length of the logitudinal semi-axis of hyperellipsoid S^*, lying on its axis of revolution WW^*, b is the length of the transversal semi-axis, $\boldsymbol{r}$ is the vector defining the location of the hyperellipsoid centre and axis WW^*, $\boldsymbol{\mu}=\boldsymbol{r}/|\boldsymbol{r}|$ is the unit vector. The development of inelastic deformation deviators $\boldsymbol{\varepsilon}$ is controlled by the normality rule associated with (1):

$$d\varepsilon=\omega dq, \quad \omega=\operatorname{grad} f/|\operatorname{grad} f|, \quad dq=(d\varepsilon\cdot d\varepsilon)^{(1/2)}. \tag{2}$$

To simulate subsequent yield surface evolution in A.A. Ilyushin's space under tensile (ε_1) load with episodic elastic unloading, relationships of an inherited kind with the Stieltjes integrals are used:

$$a=s_0+\int_{t_0}^{t}[\alpha L_1(t-\tau)+L_3(t-\tau)]d\varepsilon_1, \tag{3}$$

$$b=s_0+\int_{t_0}^{t}\left[\beta L_2(t-\tau)+L_3(t-\tau)\right]d\varepsilon_1, \tag{4}$$

$$r=(1-\alpha)\int_{t_0}^{t}L_1(t-\tau)\,d\varepsilon_1, \tag{5}$$

$$L_1(t-\tau)=L_2(t-\tau)=p_0+p_1\exp[(-\gamma(t-\tau)], \tag{6}$$

$$L_3(t-\tau)=g\{1-\exp[(-\psi(t-\tau)\}, \tag{7}$$

where $\alpha, \beta, p_0, p_1, \gamma, g, \psi$ are material constants, t_0 is the time point of the beginning of inelastic deformation, s_0 is the radius of the initial yield surface. In (6) function L_1 characterizes the development of the workhardening relaxation effect. In (7) L_3 is the function used to simulate a well-known strain aging effect manifesting in the form of subsequent yield surface isotropic expansion in time [12].

After momentary tension at t_0=0 to inelastic deformation $\varepsilon_1^* = const$ followed by momentary elastic unloading from (3)-(7) for t>0 the following is obtained:

$$r = (1-\alpha)[p_0 + p_1 \exp(-\gamma t)]\varepsilon_1^* \tag{8}$$

taking into consideration the effect of workhardening relaxation

$$a = s_0 + \alpha\left[p_0 + p_1 \exp(-\gamma t)\right]\varepsilon_1^*, \tag{9}$$

$$b = s_0 + \beta[p_0 + p_1 exp(-\gamma t)]\varepsilon_1^*, \tag{10}$$

taking into consideration the effects of workhardening relaxation and strain aging

$$a = s_0 + \{\alpha\left[p_0 + p_1 \exp(-\gamma t)\right] + g\left[1-\exp(-\psi t)\right]\}\varepsilon_1^*, \tag{11}$$

$$b = s_0 + \{\beta\left[p_0 + p_1 \exp(-\gamma t)\right] + g\left[1-\exp(-\psi t)\right]\}\varepsilon_1^*. \tag{12}$$

4. Computer simulation of the process of experimental construction of the subsequent yield surface

Mathematical models (1), (8)-(10) and (1), (8), (11), (12) at known values of material constants gave an opportunity to develop software (module RP) that simulates the process and outcomes of experimental studies of the subsequent yield surface evolution. The software allows modelling, in particular, traditional methods of experiment fulfilment. At the same time general-purpose software PR1 has been also developed that permits to calculate material constants in (8)-(12) by minimizing deviation of theoretical points from experimental ones:

$$\min_P \sum_{i=1}^{n} \| \boldsymbol{s}^{th}(t_i) - \boldsymbol{s}^{ex}(t_i) \| \to (\alpha, \beta, p_0, p_1, \gamma, g, \psi), \tag{13}$$

where P is the set of all permissible values of the mathematical model parameters, $\boldsymbol{s}^{ex}(t_i)$ is the experimental value of the i-th local yield point at time t_i, $\boldsymbol{s}^{th}(t_i)$ is the same theoretical value. Values $\boldsymbol{s}^{th}(t_i)$ are calculated by the software according to the data provided by the method of probing local yield boundaries in the experiment (complete or partial unloading, trajectories of movement to the yield boundary at points probing, etc.). In addition, PR1 visually demonstrates evolution of the subsequent yield surface in the form of a sequence of momentary elliptic yield boundaries.

The developed software permits to check up a principal possibility to explain the reasons of occurrence of the known features of the subsequent yield surface shape in experiments and the influence of the kind of unloading on the yield surface. To do so, values t_i, traditionally missing in the description of experiments, may be set by introducing some natural assumptions. So, during computer simulation of the experiments in [3] on construction of a subsequent yield surface after a mild steel sample having been subjected to tensile loading ε = 10 % followed by complete unloading, the time $\Delta t_i = t_i - t_{i-1}$ required for probing the third and all subsequent points of tension (compression) combined with twisting was assumed to be equal to some constant Δ_*. Duration Δt_1 of obtaining the first point in the experiment (Δt_1 includes time for sample relaxation and first point probing) was introduced into the set P of the search parameters. Time Δt_2 of the second point probing was also included into P. The nearest approach of the theoretical points to the experimental data (Fig. 1) was achieved at $\Delta t_1 = \Delta_*$, $\Delta t_2 = 0.1\Delta_*$ for mathematic model (1), (8)-(10).

The obtained result revealed that in experiment [6] the time for relaxation was not enough to obtain an experimental subsequent yield surface of typical geometry (a rounded nose, flatness of the opposite section). Indeed, computer simulation of numerous tests with typical resulting subsequent yield surfaces showed $\Delta t_1 > 2\Delta_*$. For example, computer simulation of the experiment in [13] (tension up to 2 % of a sample of AL6061 – T6511 alloy, partial unloading) gave almost complete coincidence of experimental and theoretical points at $\Delta t_1 = 2.273 \max(\Delta t_2, \ldots, \Delta t_8)$.

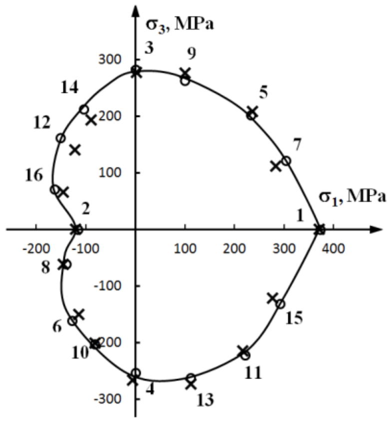

Fig. 1. Subsequent yield surface determined from complete unloading state [3]. The theory and experiment.

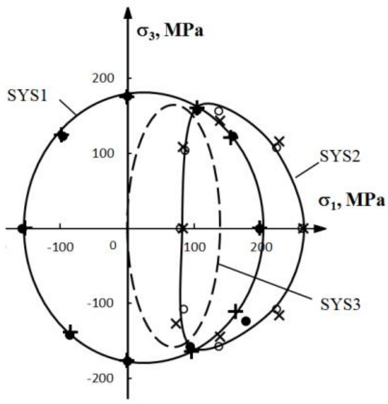

Fig. 2. Subsequent yield surfaces determined from complete unloading state (SYS1) and from partial unloading state (SYS2) [6]. The theory and experiments:
+ and ● (SYS1), × and ○ (SYS2).

Addressing the issue of influence of the kind of unloading on the shape and position of a subsequent yield surface in the space of stresses, let us look at the results of experiments (Fig. 2) [6], in which the above mentioned effect manifested itself in the most contrast manner. Figure 2 shows data received after the tension (2 %) of two identical copper samples followed by complete (SYS1) and partial (SYS2) unloading. It is obvious, that principal differences between SYS1 and SYS2 cannot be explained from the scleronomous plasticity concepts. Indeed, after complete unloading, SYS2 should have moved to the position of SYS3 with just minor changes in its shape due to low plastic straining acquired on the section of additional unloading. At the same time, the above phenomenon can be explained from the rheonomous plasticity positions. Firstly, at the "instantaneous" partial unloading the subsequent yield surface commences its relaxation movement from the point of final loading, and at the complete unloading – from the SYS3 position. Secondly, geometric differences of two subsequent yield surfaces are determined by the time of relaxation, which is selected by an experimenter for each experiment at his/her own discretion. Applying procedure (13) to all data of two tests, and including numerous variants of sequences of sample preparation and their Δt_i $(i = 1, \ldots, 18)$ into P, material constants of model (1), (8)-(10) common for both experiments were derived. At $\Delta t_{1,1} = 18\Delta t_{1,2}$ ($\Delta t_{1,1} = \Delta t_1$ of the first sample, $\Delta t_{1,2} = \Delta t_1$ of the second sample), a satisfactory approach of the theoretical points to experimental ones was achieved (Fig. 2).

5. Base experiment

A base experiment is suggested to be conducted by introducing the following changes in the traditional method of experimental study of subsequence yield surface evolution on a single sample: 1) to exclude the procedure of relaxation; 2) to repeat cyclically similar probing programme with a minimum number of points sufficient to construct a subsequent yield surface in the form of an ellipse in every cycle; 3) to record time of obtaining every boundary point; 4) to bring the first cycle as close as possible to the starting point of unloading. Then, the visual result may be presented graphically in the form of an ellipse family with indication of the average time of every cycle. To specify the procedure of identification of constitutive relations, methods of the fuzzy-set theory may be used.

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