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Investigation of the features of polycrystals complex loading using a two-level crystal plasticity theory

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Abstract. The article considers a two-level mathematical model of inelastic deformation of metal polycrystals taking into account evolution of the structure. The structure of the model was considered, some special features of its application to describe the intensity of inelastic deformations were marked. The need for a careful physical analysis of the hardening laws construction was highlighted. To evaluate the applicability of multi-level models to describe the known experimental effects of cyclic deformation a number of results of field experiments on the complex proportional and disproportional cyclic deformation was considered, some specific effects that appear in these processes were identified: stresses amplitude output at the stationary value; additional cyclic hardening at a disproportionate loading, which magnitude depends on the so-called degree of disproportionality. Numerical experiments on the disproportionate cyclic loading were carried out, the possibility of modified hardening laws to describe access to the stationary values of the stress intensity was noted, and also the possibility of a qualitative description of the effect of additional cyclic hardening was demonstrated. The A.A. Ilyushin hypothesis by isotropy and the principle of vector properties delay at the turn of the deformation path were validated.

1. Introduction

Severe plastic deformation processes (SPD) are of great concern in the modern material processing technologies, especially in production of textured sub-microcrystalline and nanocrystalline materials with high performance properties. Development of process conditions of SPD requires setting up and solving of corresponding boundary value problems of solid mechanics. The most important element in the process of setting up is formulation (or selection from existing ones) of constitutive relations (CR). From the positions of classical (macrophenomenological) solid mechanics, the materials used in SPD processes are mediums with memory [1-2], which reaction on external action is determined by their previous history of loading and its complexity. In order to execute quantitative estimation of the later the plasticity theory widely uses concepts introduced by A.A. Ilyushin (stress and strain vectors, deformation path, loading process images).

On the other side, the recent decades have shown an intensive development of approaches to building material models at the "junction" of nonlinear solid mechanics and solid-state physics. Models of this class, usually called crystal plasticity theories, are based on introduction of inner variables, i.e. parameters describing evolving meso- and microstructure of polycrystalline materials [3].

2. Materials and methods

In this paper it is considered only a two-level model of polycrystalline material. Crystallites (grains, subgrains) are the elements of lower level (mesolevel), polycrystalline aggregate (aggregation of several hundreds of crystallites) is the element of an upper level. Congeneric parameters of macrolevel and mesolevel are marked by similar letters, but congeneric parameters of macrolevel are marked by capital letters and of mesolevel – by lower-case letters.

Constitutive model for description of behavior of the representative volume of macrolevel is represented by the following combination of relations:

$$\begin{cases} \Sigma^{\mathrm{r}} \equiv \dot{\Sigma} + \Omega^{\mathrm{T}} \cdot \Sigma + \Sigma \cdot \Omega = \Pi : D^{e} = \Pi : (D - D^{in}), \\ \Omega = \Omega\left(\omega_{(i)}, \pi_{(i)}, \sigma_{(i)}\right), i = 1, \ldots, N, \\ \Pi = \Pi(\pi_{(i)}, o_{(i)}), i = 1, \ldots, N, \\ D^{in} = D^{in}(d^{in}_{(i)}, \pi_{(i)}, \omega_{(i)}), i = 1, \ldots, N, \end{cases} \tag{1}$$

where Σ – Cauchy stress tensor, Π – elasticity moduli tensor, D, D^e, D^{in} – strain rate tensor, its elastic and inelastic components, index "r" means corotation derivative which is independent from coordinate system, Ω – macro level spin; $\pi_{(i)}, \sigma_{(i)}, d^{in}_{(i)}, \omega_{(i)}, o_{(i)}$ – tensors of elastic moduli, stress tensor, inelastic component of strain rate and orientation of lattice of *i* crystallite on mesolevel, *N* – number of crystallites that create the representative volume.

The following system of relations (crystallite number omitted) is used on mesolevel of two-level model:

$$\begin{cases} \sigma^{\mathrm{r}} \equiv \dot{\sigma} - \omega \cdot \sigma + \sigma \cdot \omega = \pi : d^{e} = \pi : (d - d^{in}), \\ d^{in} = \sum_{i=1}^{K} \dot{\gamma}^{(i)} m^{(i)}_{(S)}, \\ \dot{\gamma}^{(i)} = \dot{\gamma}_0 \left| \dfrac{\tau^{(i)}}{\tau^{(i)}_c} \right|^{1/n} H(\tau^{(i)} - \tau^{(i)}_c), \ i = 1, \ldots, K, \\ \dot{\tau}^{(i)}_c = f(\gamma^{(j)}, \dot{\gamma}^{(j)}), \ i, j = 1, \ldots, K, \\ \hat{\nabla} v = \hat{\nabla} V, \end{cases} \tag{2}$$

where σ – Cauchy stress tensor, π – crystallite elastic properties fourth-rank tensor, d, d^e, d^{in} – strain rate tensor, its elastic and inelastic components on mesolevel, $\gamma^{(i)}, \tau^{(i)}_c$ – accumulated shear and critical shearing stress by *k* slip system, $\dot{\gamma}_0, n$ – material constants, $\tau^{(i)}$ – tangential strain acting in *k* slipping system, $H(\cdot)$ – Heaviside function, K – number of crystallographic systems for considered type of lattice.

In [4] the problem of matching of the defining relations of different scale levels in two-level models of inelastic deformation were considered:

$$\Pi = <\pi>, \quad \Sigma = <\sigma>, \quad D = \langle d \rangle . \tag{3}$$

It was shown that the macro spin tensor Ω and inelastic component of the strain rate tensor D^{in} should be determined by the relations:

$$\Omega = <\omega>, \tag{4}$$

$$D^{in} = <d^{in}> + \Pi^{-1} : <\pi' : d^{in\prime}> - \Pi^{-1} : (<\omega' \cdot \sigma'> - <\sigma' \cdot \omega'>), \tag{5}$$

where primes denote the deviation of the corresponding quantities from their average values for representative macrovolume.

As the basic hardening law [5-6] in $(2)_4$ the relation of the form [7] was used:

$$\dot{\tau}_c^{(k)}\left(\gamma^{(i)},\dot{\gamma}^{(i)}\right)=G\left(\sum_{i=1}^{24}a_i^{(k)}\frac{\left(\gamma^{(i)}\right)^{\psi}\dot{\gamma}^{(i)}}{\left(\sum_{i=1}^{24}\gamma^{(i)}\right)^{\delta}}\right),\ k=\overline{1,24},\ \ \psi>0,\ \gamma^{(i)}\geq 0, \qquad (6)$$

where $a_i^{(k)}$ – matrix of dimensionless hardening moduli; G – shear modulus.

3. Results

In this paper a series of experiments on the disproportionate cyclic deformation is considered, given in [8]. In [8] the disproportionate loading of the sample was considered, the type of the control signal is given below:

$$l=l_m\sin(\omega t),\ \gamma=\gamma_m\sin(\omega t-\varphi),\ \rho=\gamma_m\sqrt{3l_m}, \qquad (7)$$

where l – current sample elongation, γ – current sample twist angle, parameter φ – phase difference between the torsion and tension (in [8] φ called the degree of loading disproportionality), ρ – factor which relates the amplitudes of the two components of deformation. Under disproportionate cyclic loading increase of shear stress, depending on the degree of disproportionality of deformation is observed. The effect was named an additional hardening, and for the convenience of this additional hardening was correlated with yield strength during deformation in compression - tension. The value of additional hardening could be up to 100% of the hardening that occurs with a proportional cyclic loading.

We marked out on the stationary values of the stress intensity at the optimal choice of the parameters of the law hardening in numerical experiments (Figure 1).

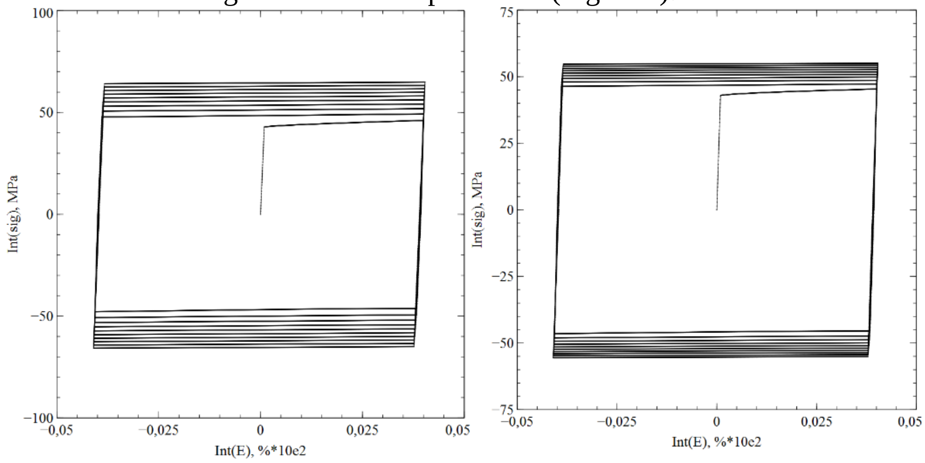

Figure 1. Dependence of the stress intensity on the strain intensity under cyclic tension - compression, 10 cycles, the law (6) is used, the parameter $\psi=1{,}3$ (on the left), $\psi=1{,}5$ (on the right).

Disproportionate cyclic loading leads to a substantial change in the structure of the material at the micro level, there is a sliding edge dislocations across multiple evolving slip systems. According to the data obtained in [8], depending on the angle disproportion φ (7) additional hardening appearing at disproportionate loading changes significantly.

Figure 2(a) represents two dependences of stress intensity on strain intensity using only the main term in the hardening law (6). It should be mentioned that further stress intensity will have a strictly positive sign, i.e. one cycle of loading corresponds to even and odd cycles in the diagram according to the intensity of the stresses and strains.

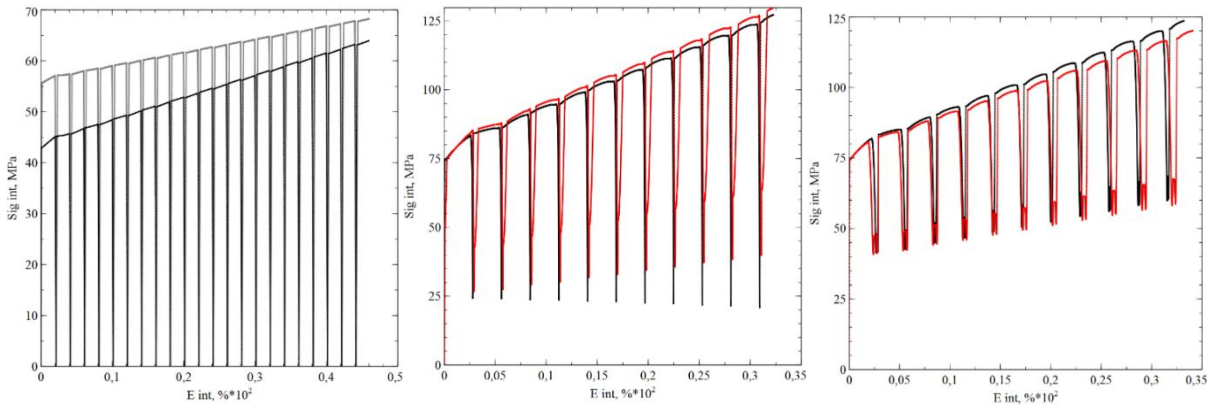

Figure 2. Dependence of the stress intensity on the strain intensity:
a) under cyclic tension - compression (gray) and shear (black), 11 cycles; b) under disproportionate cyclic loading, at values of disproportionality angle φ of 0 (black) and 15 (red) degrees; c) under disproportionate cyclic loading, at values of disproportionality angle φ of 0 (black) and 15 (red) degrees, 6 cycles.

When considering the loading diagram in Figure 2(a) it was found out that value of the stress intensity is different due to the fact that the shear is implemented different picture of edge dislocations than in tension-compression. Thus, in the tension test slip systems are oriented in such a way that the critical stresses in them have come at lower values of the stress intensity.

Figure 2(b-c) shows the results of the disproportionate loading at various disproportionate angles φ (at 0, 15, 30, 45 degrees). On the diagrams, one can see a nonlinear variation of stresses in the zone of plastic deformation. This is related to the more complex activities of slip systems in this type of loading due to the fact that the slip systems are activated depending on the value of the tangential stresses in each. It should be noted, that disproportionate loading becomes a significant change of shear stresses, and the slip system, as activation, make a comprehensive contribution disproportionate to the growth of the critical stress.

Based on the numerical experimental data table was constructed according to the stationary values of the stress intensity on the angle of disproportionality (Table 1).

Table 1. The dependence of the steady-state values of the stress intensity on the disproportionate angle.

№	φ, degrees	σ_u, MPa
1	0	79.2
2	15	79.3
3	30	79.7
4	40	80.5

Hence, it is interesting to verify fulfillment of the postulate of isotropy for the case of complex loading of representative macrolevel ("macro specimen") [9]. The following two paths are taken as two paths that differ only by their orientation in deformation space and have the same geometry:

$$1)\ \textit{stretching along axis } Э_1 \rightarrow \textit{deformation along axis } Э_3, \qquad (8)$$

$$2)\ \textit{deformation along axis } Э_3 \rightarrow \textit{stretching along axis } Э_1. \qquad (9)$$

Figure 3 represents loading process images for different deformation breaking paths (8) and (9), stress intensities marked by numbers on vector ends.

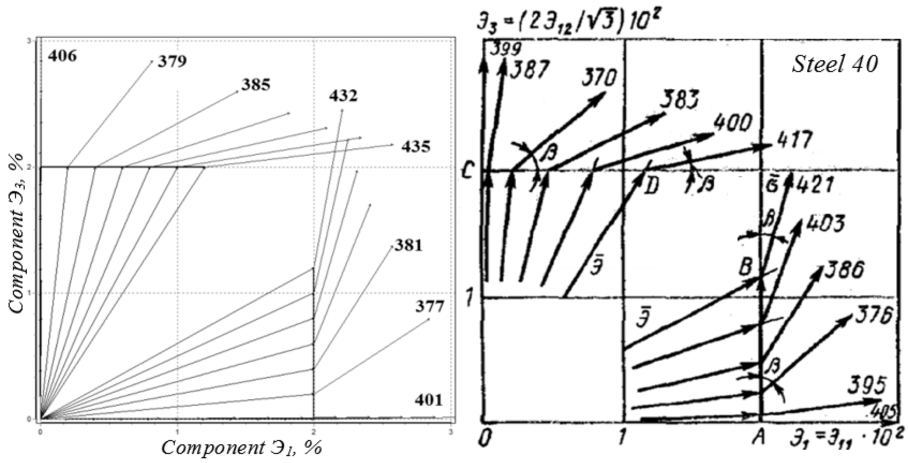

Figure 3. Process image for different deformation breaking paths (8) and (9); on the left – numerical experiment [10], on the right – natural experiment [11].

Projections of loading process images on plane $Э_1$–$Э_3$ are obtained for paths under consideration, by this projections we can judge on fulfillment of isotropic postulate, namely: before path breaking angles between stress and strain rate are the same and close to 0˚, thereat design and experimentally measured moduli of stress vector differ not more than by 1%, after path breaking angles between tangent line to deformation path and strain vectors and strain vector moduli differ not more than by 2%. Comparison of strain vector lengths shows us lowering (just about by 7-8%) of intensity of flow stress (the effect of "stress dive"). On the basis of considered information we can make a conclusion on good qualitative and quantitative conformity of vector and scalar properties established experimentally and obtained in numerical experiments [12-13].

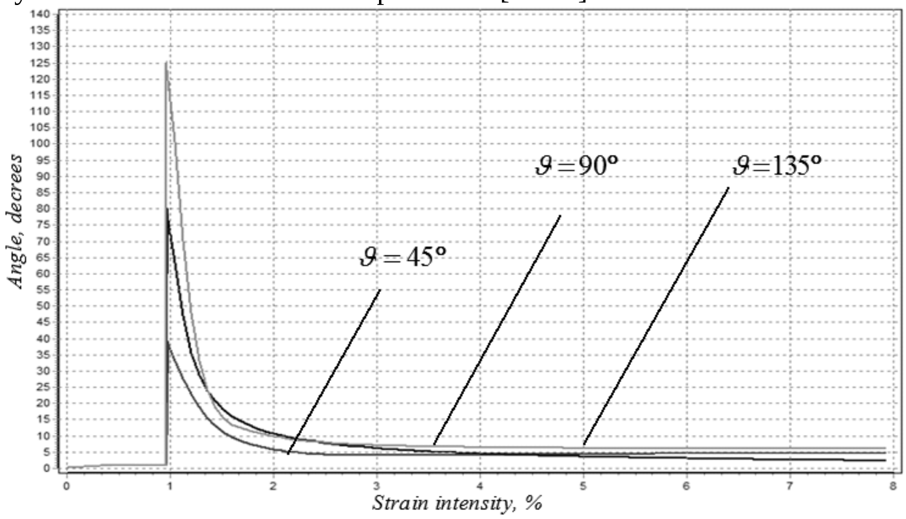

Figure 4. Dependence of the angle between stress vector and strain rate vector under different angles of deformation path breaking (numerical experiment)

Figure 4 shows results of numerical experiments that demonstrate the concept of lagging of scalar properties. Diagrams represent dependence of angle between stress vector and strain rate vector on full cumulative deformation intensity. Let us note that the data of natural experiments [12] leads to certain questions associated with the value of angle between stress vector and tangential line to path just after breaking, which is in some cases higher than the value of path breaking angle. Comparative analysis of dependences helps us to make a conclusion on good qualitative and quantitative correspondence of results, but velocity of approaching of angle to 0˚ in numerical experiments slightly differs from those that are registered in natural experiments. It is worth mentioning, that both in numerical and natural experiments the velocity of approaching the angle θ to zero almost does not depend on the value of path breaking angle: after ending of 1-2% of deformations after breaking, diagrams of dependence of angle on deformation arc length are very close.

4. Conclusions

Thus, in the article the results of a series of field experiments on the cyclic deformation were considered, some characteristics of these processes were identified. The applicability of the hardening law was validated; critical orientation in which there is linear plastic deformation was marked. The hardening law was construct that allows describing the phenomena observed in the experiments: access to the stationary value stress-strain curve. It was considered a set of numerical experiments on cyclic loading disproportionate, we noted the possibility of modified hardening law to describe access to the stationary values of the stress intensity, and also demonstrate the possibility of a qualitative description of the effect of additional hardening.

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