ZESZYTY NAUKOWE POLITECHNIKI RZESZOWSKIEJ 290, Mechanika 86
RUTMech, t. XXXI, z. 86 (4/14), październik-grudzień 2014, s. 639-649

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HARDENING LAWS IN MULTILEVEL CRYSTAL PLASTICITY MODELS AND MACRO EFFECTS OF COMPLEX CYCLIC LOADING

The problem of constructing a physically based hardening laws of mono- and polycrystalline samples in multi-level theories using crystal plasticity is considered, these hardening laws should allow describing the process of the defect structure evolution of the material due to the intensive inelastic deformations. It is also should be applicable to the description of complex and cyclic loading. An approach to the construction of a general and a particular form of hardening law is proposed, which takes into account the interaction of full and split dislocations with each other, forming and destruction of dislocation barriers, annihilation of dislocations during reverse loading and the interaction of intragranular and grain boundary dislocations. Using the obtained hardening law, the known experimental effects of complex and cyclic loading are described.

Keywords: multilevel models, crystal plasticity, hardening, complex loading, cycle loading, damage accumulation.

1. Introduction

Changes in the physical and mechanical properties of the specimen during deformation in complex cyclic path is a consequence of a substantial restructuring of the micro- and mesostructure of the material, mainly – a consequence of a significant evolution of the dislocation (wider – defective) structure of the material [1]. Directly into the structure of crystal plasticity relations description

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of the microstructure evolution is introduced through specific relationships that determine the change of the critical shear stress on the slip systems on a set of parameters defined on the basis of physical analysis (shears, temperature, stacking fault energy etc.), which are commonly called hardening law [2-4]. The above explains the considerable attention in crystal plasticity theories, which is paid to the modification of hardening law, in particular – in connection with the new experimental data obtained with the use of high-resolution equipment (in particular – an electron microscope), this is shown in [5].

The aim is to study the effects produced by polycrystalline representative macro volume of material under complex and cyclic loading (and the transition from one to another type of loading) as a consequence of changes occurring at the level of the dislocation structure in the process of loading, and attempt to modify the laws hardening so way that they can physically transparently describe these changes and effects. In particular, the unresolved issue is to justify and describe the known experimental effects, such as the dependence of additional cyclic hardening of the degree of disproportionality of loading, cyclic softening the transition from non-proportional to proportional loading, transverse reinforcement, which manifests itself when, after proportional loading in one direction is followed by proportional loading in the other direction.

2. Two-level constitutive model for inelastic deformations of polycrystals and hardening description

This paper uses a model based on the developed by a team of the Department of mathematical modeling of systems and processes Perm National Research Polytechnic University two-level approach to the consideration of inelastic deformation of polycrystalline metals (see [1]). As a top (macro-) level, we consider representative volume of the material, and the lower level means the level of the individual crystallites. Next, to simplify the upper level (macro-representative) will be called the macro level, and the lower (separate single crystals with ideal crystal lattice) will be called meso level.

The constitutive model of the macro-level is the following set of equations (hereinafter macro-parameters are indicated in capital letters, the similar meso parameters – in lower case):

$$\left.\begin{aligned}
&\boldsymbol{\Sigma}^{\mathrm{R}} \equiv \dot{\boldsymbol{\Sigma}} + \boldsymbol{\Omega}^{\mathrm{T}} \cdot \boldsymbol{\Sigma} + \boldsymbol{\Sigma} \cdot \boldsymbol{\Omega} = \boldsymbol{\Pi} : \mathbf{D}^{\mathrm{e}} = \boldsymbol{\Pi} : (\mathbf{D} - \mathbf{D}^{in}) \\
&\boldsymbol{\Omega} = \boldsymbol{\Omega}\left(\boldsymbol{\omega}_{(i)}, \boldsymbol{\pi}_{(i)}, \boldsymbol{\sigma}_{(i)}\right), i = 1, \ldots, N \\
&\boldsymbol{\Pi} = \boldsymbol{\Pi}(\boldsymbol{\pi}_{(i)}, \mathbf{o}_{(i)}), i = 1, \ldots, N \\
&\mathbf{D}^{in} = \mathbf{D}^{in}(\mathbf{d}^{in}_{(i)}, \ \boldsymbol{\pi}_{(i)}, \boldsymbol{\omega}_{(i)}), i = 1, \ldots, N
\end{aligned}\right\} \qquad (1)$$

here: $\mathbf{\Sigma}$ – Cauchy stress tensor, $\mathbf{\Pi}$ – elastic moduli tensor, $\mathbf{D}$, $\mathbf{D}^e, \mathbf{D}^{in}$ – strain rate tensor, its elastic and inelastic parts, index R means independent of reference system choice derivative [1], $\mathbf{\Omega}$ – tensor describing the motion of the moving coordinate system with respect to which the strain is determined at the macro-level; $\mathbf{\pi}_{(i)}, \mathbf{\sigma}_{(i)}, \mathbf{d}_{(i)}^{in}, \mathbf{\omega}_{(i)}, \mathbf{o}_{(i)}$ – elastic constant tensor, stress tensor, elastic and inelastic parts of strain rate tensor, spin and the orientation of *i*-crystallite, *N* – number of crystallites forming a representative macro-level.

At the meso level (the level of the crystallite) in the two-level model using the following system of relations (crystallite number is omitted):

$$\left.\begin{array}{l}
\mathbf{\sigma}^{\mathrm{r}} \equiv \dot{\mathbf{\sigma}} - \mathbf{\omega}\cdot\mathbf{\sigma} + \mathbf{\sigma}\cdot\mathbf{\omega} = \mathbf{\pi} : \mathbf{d}^{\mathrm{e}} = \mathbf{\pi} : (\mathbf{d} - \mathbf{d}^{in}) \\
\mathbf{d}^{in} = \sum\limits_{i=1}^{K} \dot{\gamma}^{(i)} \mathbf{m}_{(S)}^{(i)} \\
\dot{\gamma}^{(i)} = \dot{\gamma}_0 \left| \dfrac{\tau^{(i)}}{\tau_c^{(i)}} \right|^{1/n} H(\tau^{(i)} - \tau_c^{(i)}),\ i = 1,\dots,K \\
\dot{\tau}_c^{(i)} = f(\gamma^{(j)},\ \dot{\gamma}^{(j)}),\ i, j = 1,\dots,K \\
\text{relations for } \mathbf{\omega} \\
\text{for which from the equation } \dot{\mathbf{o}}\cdot\mathbf{o}^{\mathrm{T}} = \mathbf{\omega} \\
\text{the orientation tensor } \mathbf{o} \text{ is defined} \\
\hat{\nabla}\mathbf{v} = \hat{\nabla}\mathbf{V}
\end{array}\right\} \qquad (2)$$

where $\mathbf{\sigma}$ – Cauchy stress tensor, $\mathbf{\pi}$ – crystallite elastic moduli tensor, $\mathbf{d}$, $\mathbf{d}^e$, $\mathbf{d}^{in}$ – strain rate tensor, its elastic and inelastic parts, $\gamma^{(i)}, \tau_c^{(i)}$ – accumulated shear and the critical shear stress on the *i*-th slip system, $\mathbf{m}_{(S)}^{(i)}$ – symmetric part of the orientation tensor of the *i*-th slip system, $\mathbf{m}_{(S)}^{(i)} = \frac{1}{2}\left(\mathbf{b}_{(S)}^{(i)}\mathbf{n}_{(S)}^{(i)} + \mathbf{n}_{(S)}^{(i)}\mathbf{b}_{(S)}^{(i)}\right)$, $\mathbf{b}_{(S)}^{(i)}$, $\mathbf{n}_{(S)}^{(i)}$ – unit vectors in the direction of the Burgers vector and the normal to the slip plane; $\dot{\gamma}_0$, n – material constants: the characteristic shear rate and rate sensitivity of the material, $\tau^{(i)}$ – acting slip system shear stress, $\tau^{(i)} = \mathbf{b}_{(S)}^{(i)}\mathbf{n}_{(S)}^{(i)} : \mathbf{\sigma}$, $H(\cdot)$ – Heaviside function, K – the number of slip systems for this type of crystal lattice, $\mathbf{o}$ – tensor of the current orientation of the crystallographic coordinate system to the fixed laboratory system.

As the defining relation (equation of state) at the meso level plays rate form of Hooke's law (2_1), taking into account the geometric nonlinearity: quasi-solid movement on the meso level is associated with the rotation of the lattice (crystallographic coordinate system); in the corotation derivative of the Cauchy stress tensor appears spin tensor, characterizes the crystal lattice rotation rate.

For scale transition we used generalized Voigt hypothesis, according to which the velocity gradient of movement for each crystallite is equal to the macro-velocity gradient $\hat{\nabla}\mathbf{v} = \hat{\nabla}\mathbf{V}$. In [1], the problem of different scale levels defining relations homogenization in the two-level model of inelastic deformation is considered, one of making results is to determine the quasi-solid movement on the macro level $\mathbf{\Omega}$ and the inelastic part of the strain rate tensor at the macro level $\mathbf{D}^{in}$ to ensure homogenization conditions:

$$\mathbf{\Pi} = <\mathbf{\pi}>, \mathbf{\Sigma} = <\mathbf{\sigma}>, \mathbf{D} = <\mathbf{d}> \tag{3}$$

It is shown that for (3) in conjunction with the systems of eqs. (1) and (2) the spin $\mathbf{\Omega}$ and inelastic strain rate tensor $\mathbf{D}^{in}$ should be determined by the relations:

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

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

where the prime denotes the deviation of the corresponding values from its average values at representative macto-volume.

In the numerical implementation of the mathematical model (1)-(5) is proposed to use the Adams-Moulton scheme („predictor-corrector”), which can significantly improve the accuracy of the calculations without significantly increasing computing time (estimation in [6]). The correct description of hardening, which is an essential mechanism of the plastic deformation, allows to obtain dependence the numerical experiments which corresponding experiments, on the other hand, in the hardening laws it is inherent the description of the microstructure of the material and the laws of its evolution.

Hardening is divided into „non-oriented” and „oriented”. The first describes the hardening regardless of the direction of deformation (under this definition, processes such as the formation of the intersection of dislocations, plaits, braids, dislocation barriers), and the hardening increases the critical shear stress at once on many slip systems (or even all at once). The second is related to the accumulation of elastic energy to „pursed dislocations” (at different barrier) and this energy may be (fully or partially) released at the change of the direction of deformation. The second type, in general, can be described by the kinematic hardening, or due to simultaneous changes in the critical shear stress on the opposite slip systems.

By using the formalism of constitutive models with internal variables and two-level mathematical model of polycrystals inelastic deformation, based on the crystal elastoviscoplastic model at meso level, we received both general and particular forms of hardening laws of mono- and polycrystalline, that allow to describe the formation and destruction of dislocation barriers, the annihilation of dislocations (and so describes Bauschinger effect), and additional hardening, resulting from the interaction of intragranular and grain boundary dislocations [1]. As the basic law is considered a power hardening law in type of:

$$\left.\begin{array}{l} \dot{\tau}_{c\,b}^{(k)} = f^{(k)}\left(\gamma^{(i)}, \dot{\gamma}^{(i)}\right) = \psi E \left(\sum_{i=1}^{24} a_i^{(k)} \left(\frac{\gamma^{(i)}}{\sum_{j=1}^{24} \gamma^{(j)}} \right)^{\psi-1} \dot{\gamma}^{(i)} \right), k = \overline{1,24}, \psi > 1, \gamma^{(i)} \geq 0 \\ \tau_{c\,b}^{(k)}(0) = \tau_{c\,b0}^{(k)} \end{array}\right\} \tag{6}$$

which takes into account the interaction of forest dislocations and modified to reflect the complexity of the previous loading.

Assuming additivity of the critical shear stress rates on the slip system due to different mechanisms of hardening, the power law (6) is supplemented by terms that take into account the basic mechanisms of obstacles during plastic deformation, left out the first (power) term:

$$\begin{aligned} \dot{\tau}_c^{(k)} = f^{(k)}\left(\gamma^{(i)}, \dot{\gamma}^{(i)}\right) + f_{bar}^{(k)}\left(\gamma^{(i)}, \dot{\gamma}^{(i)}; \alpha_1^{(i)}, \alpha_2^{(i)}, \ldots, \alpha_n^{(i)}\right) + \\ + f_{annih}^{(k)}\left(\gamma^{(i)}, \dot{\gamma}^{(i)}; \beta_1^{(i)}, \beta_2^{(i)}, \ldots, \beta_m^{(i)}\right), \quad i,k = \overline{1,24} \end{aligned} \tag{7}$$

where $\alpha_1^{(i)}, \alpha_2^{(i)}, \ldots, \alpha_n^{(i)}$; $\beta_1^{(i)}, \beta_2^{(i)}, \ldots, \beta_m^{(i)}$ – sets of internal variables describing appropriate mechanisms (in general, they may take different values at each moment of deformation for different slip systems) [7]; here the term describes additional hardening due to reactions to the split dislocations, and $f_{annih}^{(k)}\left(\gamma^{(i)}, \dot{\gamma}^{(i)}; \beta_1^{(i)}, \beta_2^{(i)}, \ldots, \beta_m^{(i)}\right)$ allows to consider a decrease of the critical shear stress for reverse slip through dislocation annihilation.

An additional hardening function $f_{bar}^{(i)}$ is taken in the form of:

$$f_{bar}^{(i)}\left(\gamma_{\mathrm{SFE}}, \dot{\gamma}^{(i)}, \gamma^{(j)}\right) = \sum_{k=1}^{6} \xi_{ik} \tau_c^{(i)} \left(1 - \frac{\gamma_{\mathrm{SFE}}}{\gamma^*_{\mathrm{SFE}}}\right) \mathrm{H}\left(1 - \frac{\gamma_{\mathrm{SFE}}}{\gamma^*_{\mathrm{SFE}}}\right) \left(\int_0^t f_{bar}^{(i)} \mathrm{d}\tau + f_0^{(i)}\right)^{-1} \times$$

$$\times \dot{\gamma}^{(i)} \left(\sum_{j \neq i}^{N*} \gamma^{(j)} + \gamma_0^b \right) \mathrm{H} \left(\int_0^t f_{bar}^{(i)} \mathrm{d}\tau - \tau_{c\,fr}^{(i)} \right) \tag{8}$$

where γ_{SFE} – stacking fault energy (SFE) of the material, γ^*_{SFE} – critical SFE, beyond which this mechanism relies insignificant for this material, $N*$ – the number of slip systems, coupled to given, $\tau_c^{(i)}$ – current (full) critical stress, $\tau_{c\,fr}^{(i)}$ – critical stress for barrier destruction, γ_0^b – small constant, ξ_{ik} – material constants, taking into account the strength of each of the six types of barriers.

The equation (8) explicitly takes into account the differences in the known types of dislocation barriers and different energies of destruction (or bypass) of these barriers (with the optional parameter $\tau_{c\,fr}^{(i)}$). Oriented hardening, which is realized by „pursed" by obstacles dislocation annihilation, due to the changing the deformation direction is also considered. Details of the physics of the annihilation process and factors affecting the decrease of the critical shear stress on the slip systems as a result of the annihilation of dislocations is considered [7]. To evaluate the released elastic energy in relation to $f_{annih}^{(i)}$ an additional factor that takes into account the complexity of the loading on all of the slip systems (here is an example for the fcc lattice) is introduced:

$$f_{annih}^{(i)}(\beta_1, \beta_2, \ldots, \beta_m) = -\xi_2 \tau_{annih}^{(i)} \frac{\gamma^{(i)}}{\sum_j \gamma^{(j)}} \dot{\gamma}^{(i)} \left(\gamma^{(i+12)} + \gamma_0^a \right), \ \tau_{annih}^{(i)}\Big|_{t=0} = \tau_{c0}^{(i)} \tag{9}$$

where: γ_0^a – small constant, ξ_2 – material constant.

3. Results and discussion

In figure 1. is shown a diagram of the cyclic uniaxial loading polycrystalline aggregate using modified relations (6)-(9), the physical and mechanical parameters of the model correspond to the technically pure copper. Nonlinear effects associated with the formation and destruction of dislocation barriers do not appear in the smallness of deformations. It is clearly visible on the stationary trajectory of deformation. It should be noted that the hardening law in the form of (6) can only describe the effects of hardening associated with linear (or weakly nonlinear, depending on the ψ value) the interaction of dislocations (in the first time – the interaction of individual dislocations with various point obstacles, as well as the interaction of dislocations each own elastic stress fields). Mathematically it is possible to determine the parameters of the law (6) to obtain a substantially nonlinear form of the loading curve, but such description cannot be considered physically correct if we try to base model on the physical separation of hardening mechanisms.

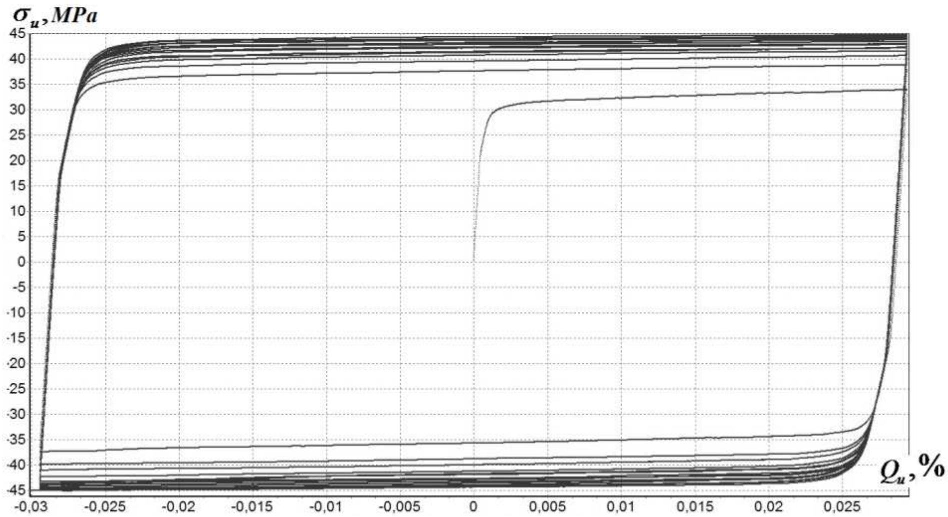

Fig. 1. The stress–strain diagram during cyclic deformation of polycrystalline aggregate; 20 cycles total

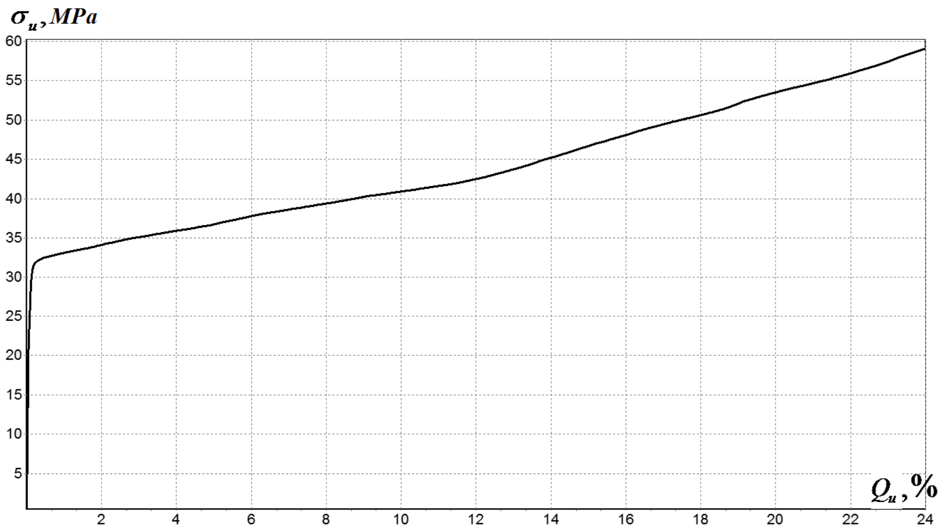

Fig. 2. The stress–strain diagram under uniaxial compression of polycrystalline aggregate; $f_0^{(i)} = 1,05$, $\gamma_0^b = 5 \cdot 10^{-5}$

Figures 2. and 3. show the dependence of various stress-strain diagram for polycrystalline aggregate if using in the hardening law additional term in the form (8), with the values specified in the caption. Clearly visible nonlinearities appearing in the diagram due to the effect of „blocking" slip systems by sessile dislocation when accumulated to a certain critical value, and accordingly releasing these systems from the deformation process. As long as there is a slip system (or set of slip systems), where the dislocation slip activate criteria is fulfilled, the material during plastic deformation will be forced to use a smaller number of slip systems than is necessary in order to fully choose the prescribed deformation. So, in the moments of one system closing and before the activate another systems the share of elastic deformation in full deformation rises sharply, resulting in a steep increase in stress on the diagram, with a further deformation there is gradual diagram alignment by activate new or additional slip systems.

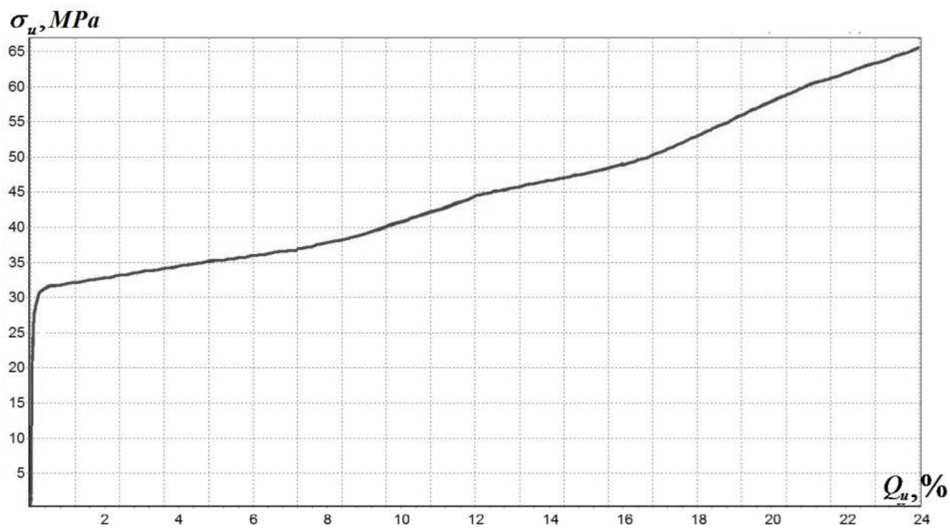

Fig. 3. The stress–strain diagram under uniaxial compression of polycrystalline aggregate, $f_0^{(i)} = 1,02, \quad \gamma_0^b = 2,5 \cdot 10^{-5}$

In addition, interesting question is the consideration of the term, which reflects the formation of sessile dislocations, depending on the concrete slip system. Figure 4. shows a typical dependence of the critical additional stress due to (8), at all slip systems randomly selected grain, on the intensity of deformation. It may be noted that very different from other systems rate of accumulation of barriers on two slip systems, which are symmetrically oriented with respect to the loading direction, in addition, a noticeable phenomenon connected deactivate and activate of slip systems process. Sharp bend at the diagram for some systems is due not so much the shear rates in these systems as the accumulation of split dislocations in a pair of conjugated systems with the highest increase of additional stresses. When activating these systems, even small shear rate on them leads to an abrupt increase in the critical stress due to the large accumulated shift in their conjugate systems. In turn, such a high increase in the critical stress leads to a rapid shutdown of the system from the plastic deformation, and the process repeats.

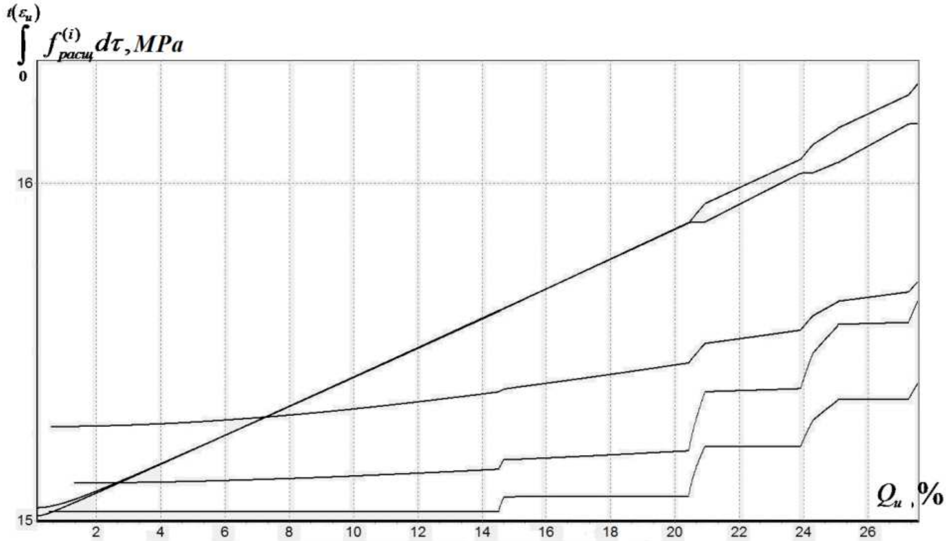

Fig. 4. Typical dependence of the critical additional stress due to (8) for the slip systems of any grain

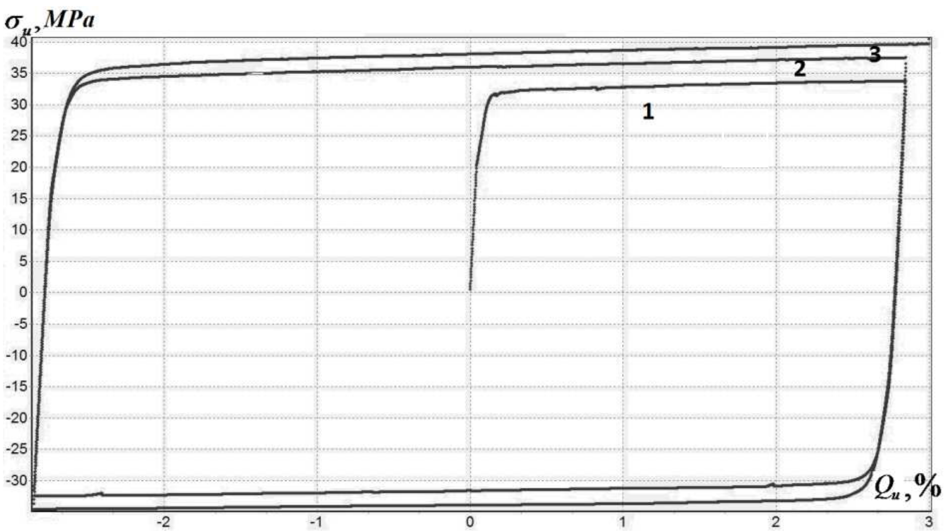

Fig. 5. The stress–strain diagram for cyclic deformation of polycrystalline aggregate with terms (8) and (9): 1-3 – cycle numbers

Figure 5. shows stress–strain diagram for polycrystalline aggregate when considering the term (9), which describes the decrease of the critical stress on the slip system, due to the annihilation of dislocations during pursed reverse loading. The calculations were performed for two cycles in tension-compression. Clearly visible reduction of the yield strength when the sign change of deformation: from 32 MPa initially to 28 MPa after the first change of deformation direction, and from 34 MPa to 30 MPa in the second cycle.

4. Conclusions

We received both general and particular forms of hardening laws of mono- and polycrystalline that allows describing the formation and destruction of dislocation barriers, the annihilation of dislocations as well as additional hardening, resulting from the interaction of intragranular and grain boundary dislocations. Thehardening is divided into „non-oriented" and „oriented". The first type describes the hardening regardless of the direction of deformation (under this definition, processes such as the formation of the intersection of dislocations, plaits, braids, dislocation barriers), and the hardening increases the critical shear stress at once on many slip systems (or even all at once). The second type is related to the accumulation of elastic energy to „pursed dislocations" (at different barrier) and this energy may be (fully or partially) released at the change of the direction of deformation. The analysis of the possible mechanisms of interaction between carriers and the plastic deformation of the crystal lattice defects is executed; hardening laws that discover a good agreement with experimental data are proposed. We also introduce the parameters characterizing the accumulation of damage and formulate fracture criterion using methodology of multilevel modelling.

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Acknowledgement

This work was supported by RFBR (grant No. 14-01-96008-r-Ural-a), the President grants No. MK-4485.2014.1, No. MК-4917.2015.1.

PRAWA UMOCNIENIA W MODELACH WIELOPOZIOMOWYCH PLASTYCZNOŚCI KRYSTALICZNEJ ORAZ SKUTKI W SKALI MAKRO ZŁOŻONEGO OBCIĄŻENIA CYKLICZNEGO

S t r e s z c z e n i e

W artykule przedstawiono problem budowy fizycznie uzasadnionych praw umocnienia próbek mono- i polikrystalicznych w wielowymiarowych teoriach plastyczności krystalicznej. Rozważane prawa umocnienia powinny pozwalać na opis procesu rozwoju struktury uszkodzenia materiału spowodowanej intensywnymi odkształceniami niesprężystymi. Powinny również umożliwiać na opis złożonych i cyklicznych obciążeń. Zaproponowano podejście do budowy ogólnej i szczegółowej postaci prawa umocnienia, które uwzględnia wzajemne oddziaływanie dyslokacji pełnych i wieloczęściowych, kształtowanie i niszczenie barier dyslokacyjnych, anihilację dyslokacji podczas procesu przeciwnego obciążania, oddziaływanie dyslokacji wewnątrzziarnowych oraz występujących na granicach ziarn. Wykorzystując otrzymane prawa umocnienia, określono znane skutki eksperymentalne złożonego i cyklicznego obciążania.

Słowa kluczowe: modele wielopoziomowe, plastyczność krystaliczna, obciążanie złożone, obciążenie cykliczne, akumulacja zniszczenia

DOI: 10.7862/rm.2014.66

Otrzymano/received: 20.07.2014 r.
Zaakceptowano/accepted: 22.11.2014 r.