Multilevel models of polycrystals using crystal plasticity: investigation of hardening laws influence on the macro effects of cyclic loading

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Abstract. 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 simple 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. Using the obtained hardening law, the known experimental effects of simple and cyclic loading are described.

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 structure of the material [1]. Describe such processes without studying and establishing appropriate mathematical models that explicitly take into account the physical root causes of the material’s microstructure evolution at large deformations. Directly into the structure of crystal plasticity relations description 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 [2-3]. 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.

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.

2. Two-level constitutive model for inelastic deformations of polycrystals
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):

\[
\begin{align*}
\Sigma^e &= \bar{\Sigma} + \Omega^e + \Sigma^e \cdot \Omega = \bar{\Pi} : \bar{D}^e \quad \bar{\Pi} : (D - D^m), \\
\Omega &= \Omega(\omega^{(i)}, n^{(i)}, \sigma^{(i)}), i = 1, \ldots, N, \\
\Pi &= \Pi(n^{(i)}, o^{(i)}), i = 1, \ldots, N, \\
D^m &= D^m(d^{m}_{n}), \quad n^{(i)}, o^{(i)}), i = 1, \ldots, N, \\
\end{align*}
\]

(1)

here \(\Sigma\) – Cauchy stress tensor, \(\Pi\) – elastic moduli tensor, \(D, D^e, D^m\) – strain rate tensor, its elastic and inelastic parts, index «R» means independent of reference system choice derivative \([1], \Omega\) – spin tensor; \(n^{(i)}, \sigma^{(i)}, d^{m}_{n}, o^{(i)}, o^{(i)}\) – 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):

\[
\begin{align*}
\sigma^e &= \bar{\sigma} - \omega \cdot \sigma + \sigma \cdot \omega = n \cdot d^e = n : (d - d^m), \\
\sigma^e &= \sum_{i=1}^{K} \sigma^{(i)} = \sum_{i=1}^{K} \left[ n^{(i)} \cdot \sigma^{(i)} \right], \\
\sigma^{(i)} &= f(\gamma^{(i)}, \Psi^{(i)}), \quad i, j = 1, \ldots, K, \\
\end{align*}
\]

(2)

here \(\sigma\) – Cauchy stress tensor, \(d, \theta, d^m\) – strain rate tensor, its elastic and inelastic parts, \(\gamma^{(i)}, \Psi^{(i)}\) – accumulated shear and the critical shear stress on the \(i\)-th slip system, \(m^{(i)}\) – symmetric part of the orientation tensor of the \(i\)-th slip system, \(n^{(i)}\) – unit vectors in the direction of the Burgers vector and the normal to the slip plane; \(\Psi, n\) – material constants: the characteristic shear rate and rate sensitivity of the material, \(\Theta^{(i)}\) – acting slip system shear stress, \(\Phi^{(i)}\) – Heaviside function, \(K\) – the number of slip systems for this type of crystal lattice, \(o\) – tensor of the current orientation of the crystallographic coordinate system to the fixed laboratory system.

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 \(\dot{\Psi}_V = \dot{\Psi}_W\).

3. Hardening model

Hardening is divided into "non-oriented" and "oriented". The first describes the hardening regardless of the direction of deformation (intersection of dislocations, plaits, braids, dislocation barriers), and a 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 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.

We received both general and particular form of hardening laws of mono- and polycrystalline, allows 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 [3].

As the basic law is considered a power hardening law in type of:

\[
\dot{\varepsilon}^{(i)} \alpha = f^{(i)}\left(\gamma^{(i)}, \Phi^{(i)}\right) = \psi E \sum_{j=1}^{24} \alpha_i^{(k)} \left(\frac{\gamma^{(j)}}{\sum_j \gamma^{(j)}}\right)^{\psi - 1}, \quad k = 1, 24, \quad \psi > 1, \quad \gamma^{(i)} \geq 0, \quad \tau^{(i)}_{c0} (0) \quad \tau^{(i)}_{c\beta}
\]

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 (3) is supplemented by terms that take into account the basic mechanisms of obstacles during plastic deformation, left out the first (power) term:

\[
\dot{\varepsilon}^{(i)} \alpha = f^{(i)}\left(\gamma^{(i)}, \Phi^{(i)}\right) + f_{\alpha}^{(i)}\left(\gamma^{(i)}, \Phi^{(i)}; \alpha_{i}^{(i)}, \alpha_{K}, \alpha_{n}^{(i)}\right) + f_{\beta}^{(i)}\left(\gamma^{(i)}, \Phi^{(i)}; \beta_{i}^{(i)}, \beta_{K}, \beta_{n}^{(i)}\right), \quad i, k = 1, 24, \quad (4)
\]

here \(\alpha_{i}^{(i)}, \alpha_{K}, \alpha_{n}^{(i)}; \beta_{i}^{(i)}, \beta_{K}, \beta_{n}^{(i)}\) – sets of internal variables describing appropriate mechanisms (in general; here the second term describes additional hardening due to reactions to the split dislocations, and third allows to consider a decrease of the critical shear stress for reverse slip through dislocation annihilation.

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

\[
f_{\alpha}^{(i)}\left(\gamma^{(i)}, \Phi^{(i)}; \gamma^{(i)}\right) = \sum_{k=1}^{6} \varepsilon_{\alpha k}^{(i)} \left(1 - \frac{\gamma^{(i)}}{\gamma_{SFE}^{*}}\right) \int_{0}^{t} \left(\int_{0}^{t} \left(\sum_{i=1}^{N} \gamma^{(i)} + \gamma_{0}^{b}\right) \left(1 + 12^{*}\right) \right) dt, \quad (5)
\]

where \(\gamma_{SFE}^{*}\) – stacking fault energy (SFE) of the material, \(\gamma_{SFE}^{*}\) – 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, \(\tau_{c\beta}\) – critical stress for barrier destruction, \(\gamma_{0}^{b}\) – small constant, \(\varepsilon_{\alpha k}\) – material constants, taking into account the strength of each of the six types of barriers.

Oriented hardening, which is realized by "pursed" by obstacles dislocation annihilation, due to the changing the deformation direction is also considered; detail 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 [3]. To account for the released elastic energy in relation for \(f_{\alpha}^{(i)}\) puts 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):

\[
f_{\alpha}^{(i)}\left(\beta_{1}, \beta_{2}, K, \beta_{n}\right) = \frac{d\tau_{\alpha}^{(i)}}{dt} = -\varepsilon_{2}^{(i)} \tau_{\alpha}^{(i)} \left(\sum_{j=1}^{N} \gamma^{(j)} \Phi^{(j)} \right) \left(\gamma^{(i)} + \gamma_{0}^{a}\right), \quad \tau_{\alpha}^{(i)}\left|_{\tau_{c0}} = \tau_{\alpha0}^{(i)} \right., \quad (6)
\]

here \(\gamma_{0}^{a}\) – small constant, \(\varepsilon_{2}\) – material constant.

### 4. Numerical results

In Fig. 1 is shown a diagram of the cyclic uniaxial loading polycrystalline aggregate using modified relations (3) – (6), 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, there do not appear in the smallness of deformations; clearly visible out on the stationary trajectory of deformation.

Fig. 2 shows stress-strain diagram for polycrystalline aggregate when considering the term (6), which describes the decreasing 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.

**Figure 1.** The stress-strain diagram during cyclic deformation of polycrystalline aggregate, 20 cycles total.

**Figure 2.** The stress-strain diagram for cyclic deformation of polycrystalline aggregate with terms (8) and (9).

Fig. 3 shows the dependence of various stress-strain diagram for polycrystalline aggregate if using in the hardening law additional term in the form (5), 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. 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.

**Figure 2.** The stress–strain diagram under uniaxial compression of polycrystalline aggregate,

a) $f_0^{(i)}=1.05$, $\gamma_0^b=5\cdot10^{-5}$, b) $f_0^{(i)}=1.02$, $\gamma_0^b=2.5\cdot10^{-5}$.

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