Polycrystalline Textures Formation

Pavel Volegov, Perm State Technical University (Perm, Russia)

I. Introduction

Crystalline bodies with ideal structure owing to unequal density of atoms in various planes and directions of a lattice possess anisotropy of some physical and mechanical properties. For example, the elastic modulus, a specific resistance, a diffusion constant have various values for different directions in a crystal. As a rule, metals and the alloys used in engineering, are polycrystals, i.e. consist of major number of the anisotropic crystal grains (grains, subgrains, etc).

In most cases in limits of representative macrovolume crystal grains statistically unordered are focused one in relation to another, therefore at a level of representative macrovolume in all directions of property it is possible to count identical then the polycrystalline body in macroscopical sense can be counted the isotropic. However if on gauges of representative volume in a spatial arrangement of such crystalline grains some orderliness the polycrystalline material will get anisotropy of properties in some allocated directions will appear. In this case usually speak about a **texture** as which understand **presence of the allocated (preferred) directions in spatial orientation of crystalline lattices of separate constituents of a polycrystalline body**.

Textures are formed owing to focused action on a body of exterior and-or interior forces. These forces can be caused by mechanical, magnetic, electrical or thermal actions, etc. Textures arise at various technological processes: crystallizations, plastic strain, etc. Important are strength properties and magnetic properties materials with textures as anisotropy of the relevant performances of a textured material is widely used in engineering.

Practically any plastic strain, except for strain under the plan of all-round squeezing, is accompanied by formation of a crystallographic texture of this or that type and this or that intensity.
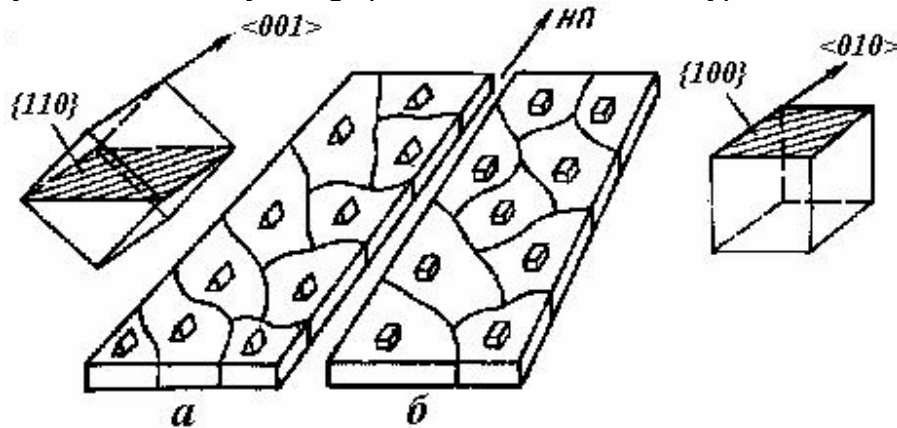

Fig. 1 the Plan of crystallographic orientation of crystal grains in a leaf material
in case of cubic *(a)* and ribbed *(б)* textures

So, for example, there is a dependence between elastic modulus E and a direction in rolled metal leafs. For many face-centered cubic lattice and body-centered lattices metals there is obviously expressed extreme E for a corner $\varphi \approx 45°$ (φ-a corner to direction of rolling and rolling plane). However character of an extreme is various.

For body-centered lattice metals it was revealed, that strength performances (σ_B and σ_T) are peak in direction rolling plane, and a protraction - in direction direction of rolling. The known phenomenon is interlinked to a texture press-effect, consisting that under certain conditions

moldings of metal their alloys strength properties in a direction of a molding appear considerably higher, than in a direction of pressing of metal also at other plans of strain (for example, at a rolling).

Thus, practical value of textures is caused by anisotropy of properties caused by them which can be rather effectively be used. In the given operation formation of textures is considered as a result of plastic strain. Interest to anisotropy on the part of experts in the field of processing metals by pressure is caused, on the one hand, by that in many cases it is important to know how it is possible to change properties and what of them with the help of plastic strain.

II. Definition and the basic methods of the description of textures

The texture is a presence of preferred orientation of separate crystal grains in a polycrystal. Usually due to presence of a texture in materials anisotropy of properties is shown. Concerning polycrystalline it is model speak, that they possess a texture in that case when crystal grains are located not quite randomly. It means, that in a sample there are some directions (or planes), along which preferentially settle down particular crystallographic direct (or planes) the crystal grains making a polycrystal.

The description of a texture is based on definition of orientation of crystal grains in some system of coordinates. The select of a system of coordinates defines an method of the description of a texture. Generally the texture of the polycrystalline unit is featured by four coordinates, three of which determine orientation, and the fourth - probability of this orientation. However the greatest distribution till the present moment three-dimensional expedients of the description of a texture (for example direct and return pole figures), that speaks smaller methodical difficulties of such description.

The description of orientation of a separate crystal

The concept of orientation is one of basic in the analysis of a texture. To describe orientation of a crystal grain, it is necessary to set its coordinate system K_{cr} (which we term as its crystallographic system of coordinates), the bound with the chosen directions in a crystal grain. At the same time in an explored sample the coordinate system of K_e (an exterior system of coordinates is inlet; we use further the term laboratory system of coordinates) which axes are the reference directions in a sample. To spot orientation of a crystal grain is means to specify the gyration translating laboratory system of coordinates K_e in crystallographic system of coordinates K_{cr}. As axes crystallographic system of coordinates K_{cr} it is the most convenient to choose directions, the bound with devices of symmetry of the best order for viewed crystalline structure. For cubic crystals as axes of K_{cr} coordinates directions of edges of a cube [100], [010], [001] are usually used. Laboratory system of coordinates also it is defined by devices of symmetry which are present at a sample; for example, for rolled leafs of an axis of coordinate system usually pick conterminous with a direction of rolling, a transverse direction and a direction of a normal line to a rolling plane. The description of gyration of coordinate systems and consequently, and the description of orientation can be carried out in several ways. The basic expedients of the description of orientation are the following:

- The Description of orientation by means of matrixes of gyration

- The Description of orientation by a corner and an axis of rotational displacement

- The Description of orientation with the help of Eulerian angles

- The Description of textures by means of pole figures

- The Description of textures by means of a distribution function of orientations

Let's consider in more detail last two expedients of the description of a texture as most frequently used on practice.

The description of textures by means of pole figures

The quantitative analysis of textures is be relative combined. It demands build-up on the received data (from X-ray patterns, etc.) special «pole figures» and their analysis. As pole figures (PF) of a polycrystal understand stereographic projections of normal lines (poles) to particular nuclear planes $\{h_i k_i l_i\}$ (i - the number of a grain), constructed for that volume of a polycrystal from which the diffraction pattern is received.

At lack of a texture any orientations of planes of different crystal grains are equality probability. In this case PF these planes represents the circle of projections uniformly covered with poles $\{h_i k_i l_i\}$. Pictorially it is accepted to figure the uniform shading of a circle of projections (fig. 2, a).
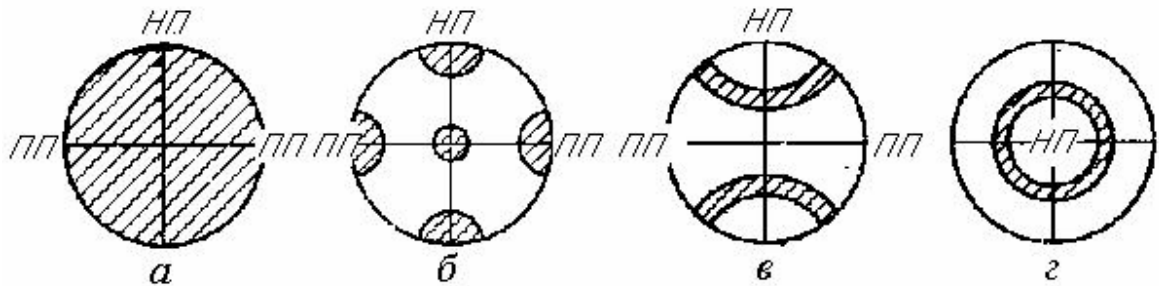

Fig. 2 Allocation of poles to pole figures for various type of textures (plan)
a- absence of a texture, δ-ideal unicomponent rolling texture (a texture of a cube, a pole figure $\{100\}$), $\emph{в}$ - an axial texture of a wire-drawing (the symmetry axis lays in a plane of a projection), $\emph{г}$ - an axial texture of a wire-drawing (the axis is perpendicular planes of a projection).

At presence of a texture of a plane $\{h_i k_i l_i\}$ different crystal grains are oriented in space by a particular natural fashion, and planes of crystal grains of one textural builders settle down so, that the relevant crystallographic parameters are focused strictly equally (if dispersion misses) or with small разориентировкой (if dispersion of a texture is).

Now the circle of projections will be covered with poles non-uniformly (fig.2, δ-$\emph{г}$). Concrete character of allocation of poles will depend on type of a texture, its dispersion and, certainly, from for what it is concrete planes $\{h_i k_i l_i\}$ is constructed given PF.

The description of textures by means of a distribution function of orientations

If represents dV plurality of volumes of all parts of a sample with orientation g in limits of a differential of orientation dg, and V - total amount of a sample,

$$\frac{dV}{V} = f(g)dg,$$

where $f(g)$ represents a distribution function of orientation of volumes of a sample (further we shall term it primely as a distribution function of orientation - DFO). This function is spotted in

orientation space φ_1, Φ, φ_2 eulerian angles where to each point the probability of presence at a sample of volume with orientation g is put in conformity. Thus, $f(g)$ completely and unequivocally features a texture of a material. Function $f(g)$ is normed so, that

$$\int f(g)dg = 1$$

(since on sense DFO there is a density function of probability).

Function $f(g)$ can be viewed as function of many variable (or function in orientation space), and the sense variable depends on an expedient of the assignment of orientation of a separate crystal grain.

III. Conceptual statement of a problem.
The purposes and problems of operation. The basic hypotheses

We will consider in this sub item of the purpose and a problem of the given operation (at the given stage of its development), and also we will formulate and we give reason for the basic hypotheses of mathematical model.

The goal of the work:

Build-up constitutive model featuring evolution of a microstructure of a material in view of the rotation modes of plasticity, for various processes of metal forming. The model should also allow to feature (qualitatively and quantitatively) process of formation in a sample - polycrystal of preferred orientations of crystalline axes of grains, that is forming the texture.

Thus:
1) At a tentative stage viewing polycrystals with face-centered cubic lattice of grains is planed;
2) Viewing is necessary possible
    а) Volume of a polycrystal with a tentative casual uniform distribution of orientations (absence of a texture);
    б) Volume of a polycrystal with some primary texture;
3) Among possible plans of a loading representing interest, such metal forming processes, as rolling and wire-drawing.

By viewing expedients of the description of textures the special attention should be given a gang independent variable with which help orientation of separate monocrystals and expedients of transition from the description of orientation of a monocrystal to the description of a texture, i.e. the description of allocation of orientations of some volume of crystal grains is featured.

The majority of the modern models of formation of textures in polycrystals is viewed with processes of turns of a polycrystal grains crystalline lattices at a microlevel, inletting concepts of dislocations of orientation discrepancy, viewing passage of systems of slip dislocations through boundary of grains at plastic strain, and relating the moments with a dislocation density of orientation discrepancy and other boundary parameters. In this paper the description of textures formation processes on mesolevel will be carried out without obvious viewing a motion of dislocations through boundaries of grains, coordinating occurrence of the moments giving in turns of grains, with discrepancy of orientations and shears on systems of slip (dislocations featuring a motion inside grains) for the next grains.

The basic hypotheses accepted by development of model, the following are:

1. The two-dimensional continuum in which to each point of a continuum the gang of coordinates in which except for spatial coordinates orientation of some allocated axis of a crystalline lattice of a grain concerning some beforehand particular axis of a laboratory system of coordinates is taken into account is put in conformity is considered.

2. To input parameters of model concern initial allocation of grains crystallographic system of coordinates orientations (the most simple expedient - a uniform distribution), the size of a grain *d*, the plan of a loading, time (or the generalized time). Target parameters - terminating allocation of orientations of grains, strain tensors components and stresses at a level of representative volume.

3. Cold plastic strain of a single-phase polycrystalline sample with face-centered cubic lattice a lattice is considered.

4. At model operation the separate grain (monocrystal) will be represented in the shape of the exact hexagon.

5. As rotational displacements of grains we shall understand here rotational displacements of crystalline lattices of grains as the whole, without fragmented structures formation.

6. Effective mechanism of plastic strain is dislocations slip on planes of crystallographic systems of slip (one or to several of three possible, fig. 3).

7. At the description of process of plastic strain of a polycrystal we would use one of models of plasticity of the polycrystal, basing on the relevant theory of plasticity for a monocrystal. Further as such theory we use model of Lin.
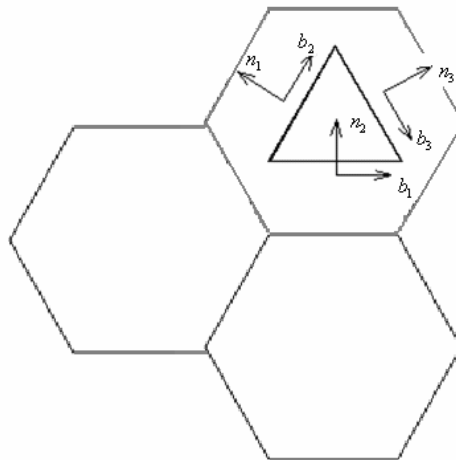

Fig. 3 Dislocations systems of slip in a two-dimensional case
for face-centered cubic lattice

Hypotheses №№ 1, 3, 4, 5 are accepted as the first approach of model and further will be omitted.

IV. Model of Lin for polycrystals

In connection with that for the description of process of an elasto-plastic deforming of representative volume (according to a hypothesis 7) it is offered to use one of physical theories of plasticity, and in the given operation - model of Lin, we stop on it more in detail and we consider substantive provisions and algorithms of this model.

The basic hypotheses:

Model of Lin is based on the following basic hypotheses:

1. Velocity of strain of the polycrystalline unit is represented by the total of elastic and plastic velocity components:
$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p, \ \dot{\boldsymbol{e}} = \dot{\boldsymbol{e}}^e + \dot{\boldsymbol{e}}^p, \ \mathrm{d}\boldsymbol{e} = \mathrm{d}\boldsymbol{e}^e + \mathrm{d}\boldsymbol{e}^p. \quad (1.1)$$

2. The complete strains of separate grains of polycrystal $\boldsymbol{\varepsilon}_{(n)}$ (n=1,2,...,N) (as well as velocities of strain) are equal to the complete strains of the polycrystalline unit:
$$\boldsymbol{\varepsilon}_{(n)} = \boldsymbol{\varepsilon}, \ \boldsymbol{e}_{(n)} = \boldsymbol{e},$$
$$\dot{\boldsymbol{\varepsilon}}_{(n)} = \dot{\boldsymbol{\varepsilon}}, \ \dot{\boldsymbol{e}}_{(n)} = \dot{\boldsymbol{e}}, \forall \mathrm{n}. \quad (1.2)$$

3. Plastic strains are isochoric, change of volume is determined by the first elastic strain invariant.

4. Plastic strains are carried out by shear on crystallographic systems of slip and submit to Shmide's law; hardening is isotropic and is defined by the total shear on all active systems of slip.

Let's consider relations of model for any way chosen grain. At presence of one active system of slip k shear $\gamma^{(k)}$ carried out in it (k) is bound to plastic strain $\boldsymbol{e}^p$ the following velocity relation:
$$\dot{\boldsymbol{e}}^p = \boldsymbol{M}^{(k)}\dot{\gamma}^{(k)}, \quad \sum_k, \quad (1.3)$$

where $\boldsymbol{M}^{(k)} = \dfrac{1}{2}\left(\boldsymbol{n}_0^{(k)}\boldsymbol{b}_0^{(k)} + \boldsymbol{b}_0^{(k)}\boldsymbol{n}_0^{(k)}\right)$ - an orientation tensor of system of slip, $\boldsymbol{n}_0^{(k)}$ - a unit vector

of a normal line of a slip plane, $\boldsymbol{b}_0^{(k)} = \dfrac{\boldsymbol{b}^{(k)}}{|\boldsymbol{b}^{(k)}|}$ - the normalized Burgers vector.

At activization of several systems of slip velocity of a deviator of plastic strain is determined by expression:
$$\dot{\boldsymbol{e}}^p = \sum_{k=1}^{K} \boldsymbol{M}^{(k)}\dot{\gamma}^{(k)}, \quad (1.4)$$

where K is the number of the active systems of slip. Activization of system of slip k is determined by performance in it of Shmide's law
$$\boldsymbol{s} : \boldsymbol{n}_0^{(k)}\boldsymbol{b}_0^{(k)} = \tau_c^{(k)}, \quad (1.5)$$

where $\boldsymbol{s}$ - a deviator of a stress tensor.

According to a hypothesis 4 critical shift stresses in each system of slip are identical and depend on the total shear:

$$\tau_c^{(k)} = \tau_c = f\left(\sum_k \int \left|d\gamma^{(k)}\right|\right). \ (1.6)$$

Velocities of elastic strains in a grain can then be spotted a relation:

$$\dot{e}^e = \dot{e} - \sum_{k=1}^{K} M^{(k)} \dot{\gamma}^{(k)}. \ (1.7)$$

With the help (1.7), using the velocity shape of a Hooke's law, it is easy to receive expression for velocity of stresses:

$$\dot{\sigma} = 2G\dot{e}^e = 2G\left[\dot{e} - \sum_{k=1}^{K} M^{(k)} \dot{\gamma}^{(k)}\right] \quad (1.7\,')$$

Velocities of elastic shift strains in k system of slip are equal to:

$$\dot{\gamma}^{e(k)} = M^{(k)} : \left[\dot{e} - \sum_{j=1}^{K} M^{(j)} \dot{\gamma}^{(j)}\right], \ (1.8)$$

and the relevant shift stresses are defined as

$$\tau_{(k)} = 2G\gamma^{e(k)} = 2GM^{(k)} : \left[e - \sum_{j=1}^{K} M^{(j)} \gamma^{(j)}\right]. \ (1.9)$$

The formula (1.9) can be copied in the velocity shape

$$\dot{\tau}_{(k)} = 2G\dot{\gamma}^{e(k)} = 2GM^{(k)} : \left[\dot{e} - \sum_{j=1}^{K} M^{(j)} \dot{\gamma}^{(j)}\right]. \ (1.9\,')$$

Let's consider process of a loading in space of strains. During the initial moment $\mathbf{e}_0 = \mathbf{0}$. At increase $\mathbf{e}$ (on quantity of intensity) in the beginning the deforming is carried out by an elastic scheme down to achievement in some system of slip (for example, with the number 1) the shift stress equals on the module to initial critical stresses $\tau_{c0} = f(0)$. After that moment inelastic slide on system 1 begins at incremental strain $\dot{e} > 0$. Thus during each moment of a deforming the requirement of plastic yielding should satisfy

$$\tau^{(1)} = \tau_c = f\left(|\gamma_1|\right),$$

or

$$2GM^{(1)} : \left[\dot{e} - M^{(1)} \dot{\gamma}^{(1)}\right] = \dot{f}\left(|\gamma_1|\right) = \frac{\partial f}{\partial \gamma_1} \dot{\gamma}_1 \quad (1.10)$$

At performance (1.10) and incremental strain $\mathbf{e}$ single shear is prolonged until in some other system of slip (for example, 2) shift stresses $\tau^{(2)}$ not achieve critical value $\tau_c = f(|\gamma_1|)$. From this time, increase $\mathbf{e}$ causes double slide on systems 1 and 2, thus a requirement should satisfy:

$$\tau^{(1)} = \tau^{(2)} = \tau_c = f(|\gamma_1| + |\gamma_2|)$$

or

$$2GM^{(1)} : \left[\dot{e} - \sum_{i=1}^{2} M^{(i)} \dot{\gamma}^{(i)}\right] = 2GM^{(2)} : \left[\dot{e} - \sum_{i=1}^{2} M^{(i)} \dot{\gamma}^{(i)}\right] = \dot{f}\left(|\gamma_1| + |\gamma_2|\right) = \frac{\partial f}{\partial (\gamma_1 + \gamma_2)} (\dot{\gamma}_1 + \dot{\gamma}_2)$$

(1.11)

Similarly involving in slide of 3-rd, 4-th and 5-th systems of slip is considered. Thus on each of the active systems of slip the requirement of fluidity (Shmide's law) should satisfy. Guessing, that in each slip plane (along one direct) answer the "positive" and "negative" direction of slide various numbers of systems of slip, it is possible to write down these requirements as follows:

$$2G\boldsymbol{M}^{(i)} : \left[\dot{\boldsymbol{e}} - \sum_{k=1}^{K} \boldsymbol{M}^{(k)} \dot{\gamma}_k \right] = \dot{f}\left(\sum_{k=1}^{K} \int d\gamma_k \right), \quad i = \overline{1, K}, \qquad (1.12)$$

Where, $\dot{\gamma}_{(k)}$, $d\gamma_k$ are non-negative, K=1,2, …, 5 - number of the active systems of slip.

For transition to model of a polycrystal one of known approaches to averaging (is used as probable variants it is possible to offer orientation averaging, or averaging on volume, or (for stresses) on a surface of representative volume).

V. Mathematical statement of a problem

In the given section we build concrete mathematical relations on which the algorithm of numerical calculations of mathematical model will be based.

For the description of orientation of crystallographic lattices of grains the distribution function of orientations (DFO) f (Ω) is used.

In a two-dimensional case orientation is determined by one corner - a corner between the chosen axis of a crystallographic system of coordinates e_1 and an axis of laboratory system of coordinates e_1', this corner we designate φ. Then the orientation space will be plurality of all values φ in limits $\varphi \in \left[0, \dfrac{\pi}{3} \right]$ (in view of symmetry of a lattice), then $f(\Omega) = f(\varphi)$. In case of a uniform distribution of orientations $f(\varphi) = const = \dfrac{3}{\pi}$.
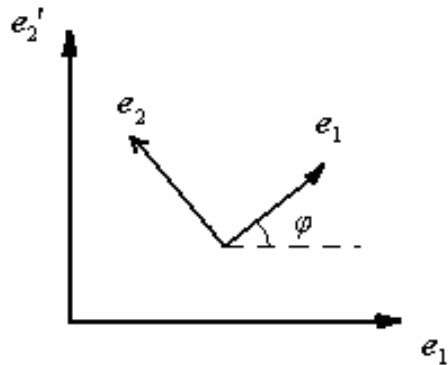

Fig. 4 the Arrangement of axes laboratory system of coordinates and axes crystallographic system of coordinates

Further it is necessary to construct the relations, allowing to expect changes of orientation of grains (depending on current orientation and from a loading).

According to the basic hypotheses of model, we shall count, that the moment developing a crystalline lattice of grains, appears on grains boundary at passage of dislocations through boundary (at plastic strain) and it is caused by various orientation crystallographic system of coordinates of the next grains generator boundary. Radiating from this, one of the arguments, quantity of the moment, the off-orientations measure the next grains $r = r(\varphi_1, \varphi_2)$, where φ_1, φ_2 - orientations of the next

grains is influencing. We impose on a off-orientations measure a normalize requirement $r \in [0,1]$, and at absence off-orientations $\Delta\varphi = |\varphi_1 - \varphi_2| = 0 \Rightarrow r = 0$, and $\Delta\varphi = |\varphi_1 - \varphi_2| = \dfrac{\pi}{6} \Rightarrow r = 1$. The last follows from properties of symmetry for face-centered cubic lattice lattices $\varphi_1, \varphi_2 \in \left[0, \dfrac{\pi}{3}\right]$.

Since in each of grains operates on three systems of slip, and, generally speaking, for the complete description of orientation of systems of slip of the fixed grain it is possible to set orientation of the arbitrary system of slip $\varphi \in \left[0, \dfrac{\pi}{3}\right]$ (orientations of the others then are equal $\varphi \pm \dfrac{2\pi}{3}$) then as a off-orientations measure it is possible to pick

$$r(\varphi_1, \varphi_2) = |\sin 3\Delta\varphi| = \sin 3|\varphi_1 - \varphi_2|. \qquad (2.4)$$

Now the primary goal of model is definition moments stresses μ and build-up of moments yielding functions $f_\mu(\mu)$ for the arbitrary grain with orientation $\varphi*$.

Let's consider (according to a hypothesis 8), that quantity of the moment incipient as a result of interaction of the given system of slip of a concrete grain with systems of slip next, is influenced also with quantity of shear on the given system of slip as a result of plastic strain i.e. as already it was spoken earlier, shall relate occurrence of such moment to a motion of dislocations in grains on the relevant systems of slip. Then we shall present the component of the moment incipient as a result of shear on i to system of slip, effective on volume with some fixed orientation $\varphi*$, on the part of volumes with other orientations (in that specific case - the next grains) as

$$\mu_i* = \mu_i*(r_i*, \gamma_i*) = a\gamma_i* \int_0^{\frac{\pi}{3}} f(\varphi) |\sin 3(\varphi_i* - \varphi)| d\varphi, \qquad (2.5)$$

where

γ_i* - shift as a result of strain on system of slip of the allocated volume with orientation $\varphi*$ (here it is necessary to note, that according to model of Lin shears on systems of slip occur as γ_i* as a result of plastic $\gamma_i^{(e)}*$, and elastic strain $\gamma_i^{(p)}*$, therefore here under can be meant both, and, depending on what strain is implemented at present loadings in the given system of slip of the given grain),

a - some dimensionless parameter, which selection of values is, generally speaking, a separate problem, $a > 0$, and further we shall consider, that the parameter and is interlinked to an elastic modulus (and defines by elastic response of a lattice of a grain as a result of the constrained shear),

i - the number of system of slip in volume with orientation $\varphi*$.

The formula (2.5) we shall write down as well in the velocity shape:

$$\dot{\mu}_i* = \dot{\mu}_i*(r_i*, \dot{\gamma}_i*) = a\dot{\gamma}_i* \int_0^{\frac{\pi}{3}} f(\varphi) |\sin 3(\varphi_i* - \varphi)| d\varphi, \qquad (2.5\text{ '})$$

Quantity of shear in concrete system of slip is defined by the law of plastic yielding or from the physical theory of plasticity, and the complete velocity moments stresses then pays off as

$$\dot{\mu}^* = \sum_{i=1}^{n} \dot{\mu}_i \,*. \qquad (2.6)$$

Let's build now relations of model, using a formalism of the theory of plastic yielding:

- We consider, that velocities of rotational displacements $\dot{\varphi}$ for the given grain can be presented as the total elastic (reversible) and plastic (nonreversible) components:
$$\dot{\varphi} = \dot{\varphi}^{(e)} + \dot{\varphi}^{(p)}, \qquad (2.7)$$

- We consider further, that elastic velocities making rotational displacements are linearly interlinked to moments stresses velocities:
$$\dot{\varphi}^{(e)} = A\dot{\mu}, \qquad (2.8)$$

- Thus for a plastic component of velocities of rotational displacements (by analogy to the theory of plastic yielding) we can write down measure of yielding:
$$f_\mu(\mu) = \mu_0, \quad (2.9)$$

And at $f_\mu(\mu) < \mu_0$ plastic change of an angle of rotation does not occur.

- Then it is possible to write down velocity of plastic rotational displacement with the help moments yield function:
$$\dot{\varphi}^{(p)} = \dot{\lambda}^{(p)} \frac{\partial f_\mu(\mu)}{\partial \mu}, \quad (2.10)$$

where $\dot{\lambda}^{(p)}$ - coefficient of proportionality.

We will be spotted now with moments yield function $f_\mu(\mu)$. By virtue of that plastic rotational displacements of crystalline lattices of grains will begin not at any values μ^*, and at excess of the certain critical value by it (in analogy to the beginning of nonreversible plastic strains) it is necessary to write down

$$\dot{\varphi}^{(p)} = \dot{\lambda}^{(p)} \left. \frac{\partial f_\mu(\mu)}{\partial \mu} \right|_{\mu=\mu_0}, \qquad (2.11)$$

And critical value μ_0 we shall calculate as follows:

$$\mu_0 = \beta \tau_0, \quad (2.11\ ')$$

Where

$\mu_0, N \cdot m / m^3$ - critical value of the moment on boundary,

τ_0, Pa - a yield strength,

β - the dimensionless dropping coefficient,

As physical backgrounds for a select of measure of activization as (2.11 ') it is possible to state the following:

First, by virtue of a hypothesis about the contribution of boundaries of grains to embodying the rotation mode we consider, that the mechanism of gyration is implemented due to plastic shears on boundaries of grains;

Second, critical stresses for shift strain on boundary are lower, than in "interior" of a monocrystal, by virtue of a boosted free energy of dislocations in boundaries;

Let's explain measure of activation (2.11 ') on a prime example of a two-dimensional grain of the exact shape. At monotonously incremental strain, as a result of interaction of the next grains on boundaries, on a viewed grain operate incremental moments stresses, within the framework of

model (and according to ideology of Cosserat continuum) grains carried to all volume (i.e. considered as the distributed on volume). Thus resistance to rotational displacement on the part of the next grains the same as also the moment μ^*, grows from zero and up to the limiting value μ_0^* which is defined from a requirement, that in each point of boundary the limiting stresses of shear $\beta\tau_0$ (occurrence of dropping coefficient β is explained above) is achieved.

During development of model the hypothesis expressed necessity of entering into measure of a standard of a diversion of the shape of a grain from the ideal shape (if to represent grains ellipsoids as such a measure the relation half-axles is possible to choose) also, however within the framework of the given, simplified variant of operation of necessity of introduction of such coefficient there is no valid a hypothesis about the identical sizes and the shape of grains. Introduction of coefficient of asymmetry, most likely, is required at the further complication of model (by viewing grains of the various size and geometry).

Let's consider a procedure of carrying out of numerical calculations by means of mathematical relations of model:

1. We shall consider the two-dimensional representative volume consisting of a plenty (approximately 1000) separate grains - monocrystals, the given the Cartesian axials (renumbered according to some rule: to a grain the double number, the first - the number horizontal, second - a vertical stratum, and a grain of even and odd stratums as on a vertical is appropriated, and across biased be relative each other on half of size of a grain by virtue of that grains completely area of model operation), and to each of grains we shall put in conformity a certain orientation $\varphi^{(ij)}$, i,j - the number of a current grain, $\varphi^{(ij)} \in [0, \dfrac{\pi}{3})$ (fig. 5).

As orientation $\varphi^{(ij)}$ we shall understand orientation of one of systems of slip ($\varphi^{(ij)}$-a corner between a trace on a plane of model operation of the system of slip nearest to an abscissa axis and most this axis; thus it is not taken into account directions of slide in this crystallographic system), such, that $\varphi^{(ij)} \in [0, \dfrac{\pi}{3})$. Then, obviously, the positive directions of other systems of slip can be written down as $\varphi^{(ij)} + \dfrac{2\pi}{3}$, $\varphi^{(ij)} - \dfrac{2\pi}{3}$
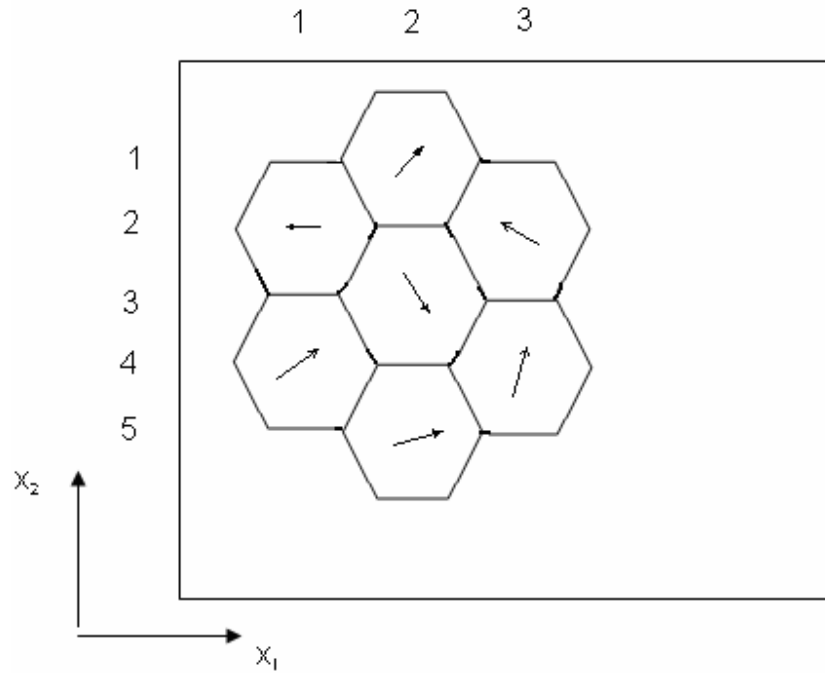
Fig. 5 the Plan of numbering of grains in representative volume, by arrows
orientations of systems of slip are designated

2. By virtue of that in model for the description of processes of an elasto-plastic deforming model of Lin is applied, we conduct process on strains, including their identical to each grain. On each step of algorithm we shall give strains some small (but finitesimal) a increment

$$\Delta e = \Delta e^* = \begin{pmatrix} \Delta e_{11} & \Delta e_{12} \\ \Delta e_{12} & \Delta e_{22} \end{pmatrix}, \qquad (3.1)$$

Here $\Delta e = \Delta e^*$ means, that the increment of strain is identical to all grains with the arbitrary orientation φ^*.

3. On initial iteration we shall set values of critical shift stresses $\tau_c^{(0)}$ and the law of hardening $\tau_c^{(k)*} = \tau_c^{(k)*}\left(\tau_c^{(0)}, \gamma^{(k)*}\right)$, where $\gamma^{(k)*}$ - the total shear on systems of slip in a grain φ^* on a step of a loading k, $\gamma^{(k)*} = \sum_{i=1}^{3} \gamma_i^{(k)*}$, i - the system of slip number. The law of hardening we shall set as

$$\tau_c^{(k)*} = \tau_c^{(0)} + \alpha E \gamma^{(k)*}, \qquad (3.2)$$

where E - an elastic modulus of a material, $\alpha \in [0,1]$ - dropping coefficient.

4. Further on a settlement step k we shall calculate necessary parameters of an elasto-plastic loading, using for this relation models of Lin (section 3.1). For transition from records of expressions in velocities to record for increments we shall use the plan of integration of Euler. Then we shall receive the following relations:
   - For the active systems of slip Shmide's law as (1.5) is carried out, and shears on the active systems of slip are defined by a principle of a minimum of shear of Taylor (1.13):

$$\sum |\Delta \gamma_i| \leq \sum |\Delta \gamma_i^*|, \qquad (3.3)$$

$i = \overline{1,2}$ - the number of the active system of slip.

Besides for the active systems of slip the tangential stresses in them (for the given grain on the given settlement step) are equal to the relevant stresses of shear $\tau_{(i)}^{(k)}* = \tau_c^{(k)}*$.

• For systems of slip on which Shmide's law is not carried out, the increment of is calculated under the formula (1.8):

$$\Delta \gamma_i^e = M^{(i)} : \left[\Delta e - \sum_{j=1}^{K} M^{(j)} \Delta \gamma_j \right], \qquad (3.4)$$

K - The number of the active systems of slip, and shift stresses are equal these systems of slip, according to (1.9)

$$\Delta \tau_{(i)} = 2G M^{(i)} : \left[\Delta e - \sum_{j=1}^{K} M^{(j)} \Delta \gamma_j \right]. \qquad (3.5)$$

The increment of a stress tensor $\sigma*_{(k)}$ in a grain $\varphi*$ on a settlement step k is defined according to a Hooke's law:

$$\Delta \sigma*_{(k)} = 2G \Delta e_{(k)}^{(e)} = 2G \left[\Delta e - \sum_{j=1}^{K} M^{(j)} \Delta \gamma_j \right]. \qquad (3.5\,')$$

Thus, on a settlement step k it is possible to calculate increments of shears on systems of slip, thus, using the relevant values for shears from the previous step to spot new values of shears (and the total shear):

$$\gamma^{(k)}* = \sum_{i=1}^{3} \gamma_i^{(k)}* = \sum_{i=1}^{3} \left(\gamma_i^{(k-1)}* + \Delta \gamma_i^{(k-1)}* \right), \qquad (3.6)$$

and also to count critical values of shears $\tau_c^{(k)}* = \tau_c^{(k)}* \left(\tau_c^{(0)}, \gamma^{(k)}* \right)$.

5. Now, using relations of section 3.2, we shall expect increments the moment stresses effective on a grain as a result of interaction of system of slip of a grain $\varphi*$ with systems of slip i of the next grains, and the complete values of the moments (2.9, 2.10):

$$\Delta \mu_i^{(k)}* = \alpha \, \Delta \gamma_i^{(k)}* \frac{1}{6} \sum_{m=1}^{6} | \sin 3(\varphi* - \varphi^{(m)}) |, \qquad (3.8)$$

$$\Delta \mu^{(k)}* = \sum_{i=1}^{3} \Delta \mu_i^{(k)}*,$$
$$\mu^{(k)}* = \mu^{(k-1)}* + \Delta \mu^{(k)}* \qquad (3.9)$$

6. In conformity with a formalism of the theory of plastic yielding, a increment of a off-orientations corner in grains we shall present as (see 2.5):

$$\Delta \varphi^{(k)}* = \Delta \varphi^{(k)(e)}* + \Delta \varphi^{(k)(p)}*, \qquad (3.10)$$

where

$$\Delta \varphi^{(k)(e)}* = A \Delta \mu^{(k)}*, \qquad (3.11)$$

and

$$\Delta \varphi^{(k)(p)}* = \Delta \lambda^{(p)} \left. \frac{\partial f_\mu(\mu)}{\partial \mu} \right|_{\mu = \mu_0}. \qquad (3.12)$$

7. Now, for final terminating a settlement step, we calculate the complete values of corners off-orientations

$$\varphi^{(k)}* = \varphi^{(k-1)}* + \Delta\varphi^{(k)}*. \quad (3.13)$$

8. Thus, in the end of each settlement step shears on systems of slip of each grain, builders of a stress tensor of a grain, the moment, the distributed on a grain and value of a corner off-orientations each grain are defined. Having applied further procedure of averaging of stresses on orientation volume:

$$\Delta\sigma_{ij} = \frac{1}{V}\sum_{k=1}^{N}V_{ij}\Delta\sigma_{ij}^{(k)},$$

where $\Delta\sigma_{ij}^{(k)}$ - a increment a builder of a tensor of strains the grain k which have been written down in laboratory system of coordinates, we shall describe tensely - deformed a state of representative volume.

VI. Results of operation

Let's give values of parameters of the model used in numerical experiments:

$$N = 1000,$$
$$G = 200 \cdot 10^6 \, \Pi a,$$
$$v = 0.316,$$
$$\tau_0 = 0.01 \cdot 10^6 \, \Pi a,$$
$$b = 2.56 \cdot 10^{-10} \, \text{м},$$
$$R* = 10^4 b,$$
$$\alpha = 0.005,$$

where
G, v - a shear modulus and Poisson coefficient,
b - the module of Burgers vector,
$R*$ - the size of a grain,
N - number of grains in representative volume,
τ_0 - an initial yield strength of a material,
a, β, α - parameters of model.

The data correspond to parameters for copper.

We consider results of evaluations for a case of strain of an axial compression along an axis e_1 of a laboratory axis of coordinates representative volume, thus we view strains of intensity from up 10^{-5} to $0,85$:
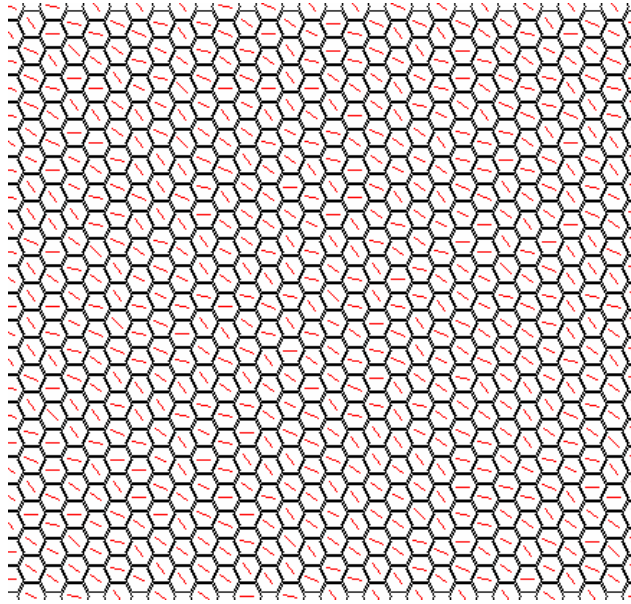
Fig. 6 Initial allocation of orientations

(a fragment of simulated area, arrows show orientation of grains $\varphi \in \left[0, \dfrac{\pi}{3} \right)$)

As target parameters of model terminating orientations of grains of representative volume act. To consider dynamics of change of orientations of grains depending on intensity of strains, we shall observe of change of an off-orientations average angle grains

$$\overline{\varphi} = \frac{1}{N} \sum_{i=1}^{N} \varphi_i$$

And mean square deviation of off-orientations corners

$$D(\varphi) = \frac{1}{N^2} \sum_{i=1}^{N} \left(\varphi_i - \overline{\varphi} \right)^2$$

Then in requirements of the given numerical experiment we received:
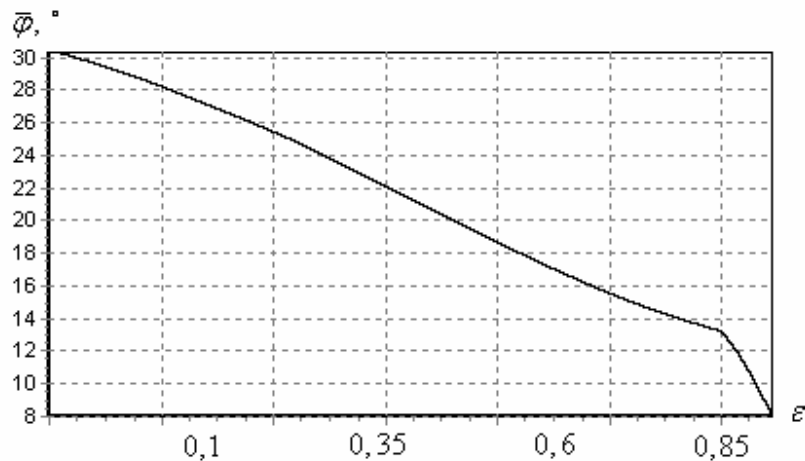
Fig. 7 Dependence of an off-orientations average angle of grains in representative volume $\overline{\varphi}$ from intensity of strains ε ($a = 0,5 \cdot 10^{-2}, \beta = 0,7$)
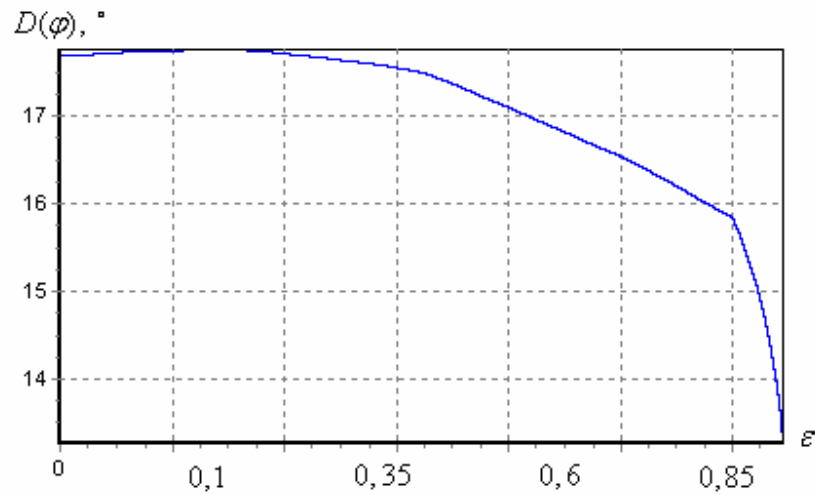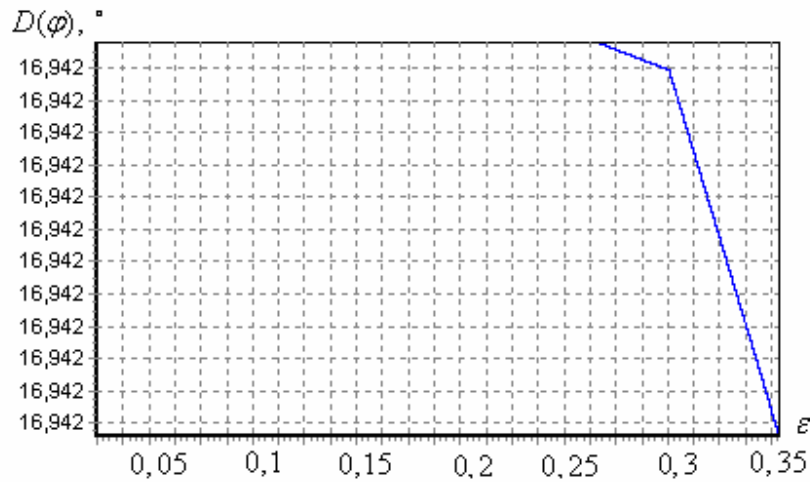
Fig. 8 Dependence mean square deviation off-orientations of grains in representative volume $D(\varphi)$ from intensity of strains ε ($a = 0,5 \cdot 10^{-2}, \beta = 0,7$)
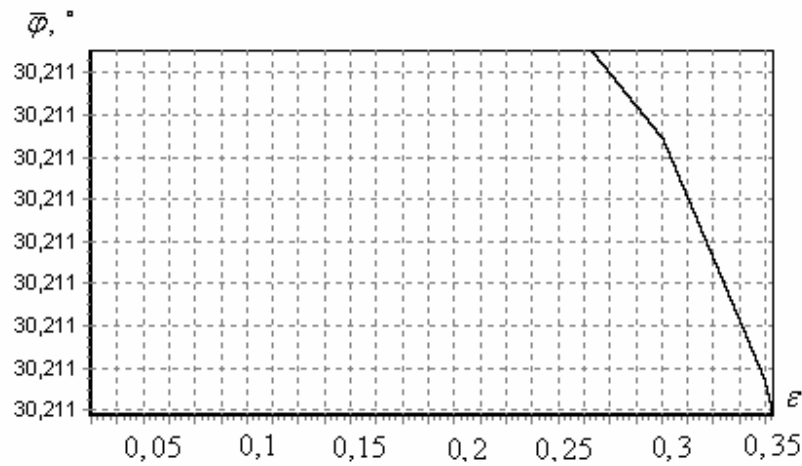
Fig. 9 Dependence of an off-orientations average angle of grains in representative volume $\bar{\varphi}$ from intensity of strains ε ($a = 0,2 \cdot 10^{-2}, \beta = 0,4$)

Fig. 10 Dependence mean square deviation off-orientations of grains in representative volume $D(\varphi)$ from intensity of strains ε ($a = 0,2 \cdot 10^{-2}, \beta = 0,4$)

In experiments which results are mapped on fig. 7-8 and fig. 9-10, the behaviour of representative volume surveyed at various values of parameters of model a and β. Having carried out the brief analysis of the submitted results, it is possible to draw a deduction, that in the given example we have the right to speak about texture formation within the framework of representative volume since at major strains there are preferred orientations, in this case – orientations $\varphi_i = 0$. Occurrences of such preferred orientation in this case could be expected radiating from symmetry of a loading (only lengthways e_1) and that fact, that orientation crystallographic system of coordinates of a grain considers orientation of system of slip, for which $\varphi^{(ij)} \in [0, \frac{\pi}{3})$. In this case, obviously, the most favourable to grains will be the orientation conterminous to an axis of a loading owing to what turns at which there is a relaxation moments stresses on boundaries begin with some moment and. In this case it is such turns at which there is, first, a grains off-orientation minimization, and second, systems of slip symmetrize in relation to main axes of a loading.
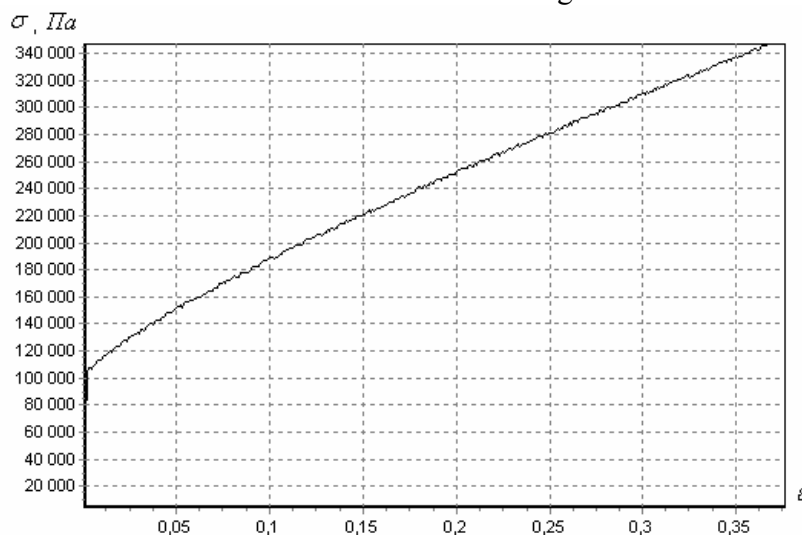
Fig. 11 Dependence of intensity of stresses σ in representative volume from intensity of strain ε ($a = 0{,}5 \cdot 10^{-2}, \beta = 0{,}7$), coefficient of hardening $\alpha = 0{,}01$
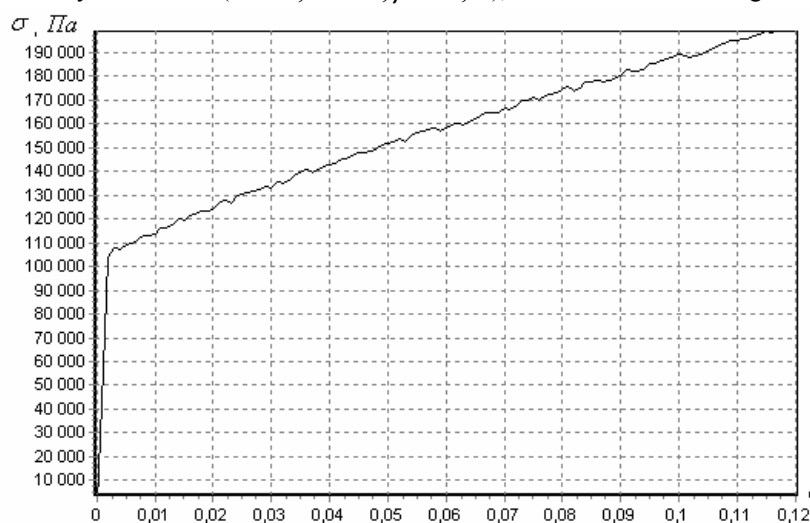
Fig. 12 Dependence of intensity of stresses σ in representative volume from intensity of strain ε ($a = 0{,}5 \cdot 10^{-2}, \beta = 0{,}7$), coefficient of hardening $\alpha = 0{,}01$

Let's note also features of behaviour of representative volume on fig. 11-12. First, we shall note, that on diagrams the site of only elastic strain which yet does not give in essential change of angles of rotation is distinctly traced. Then slide of dislocations on systems slide begins, however during even some continuance of a loading of plastic rotational displacements does not occur. Really, on this "transition" site on boundaries of grains stresses, the bound with discrepancy of crystallographic systems of slip of neighbours collect, but owing to "small" shears these stresses are still insufficient for the beginning nonreversible plastic rotational displacements. At the further magnification of strains the increasing number of systems of slip of various grains, and gradually process of rotational displacements in all grains enter process of plastic strain becomes nonreversible. At a plastic relaxation owing to rotational displacements there is a slope of stresses on a site of plasticity of the $\sigma - \varepsilon$ diagram.

The establishment of grains or conglomerates of grains with which naturally inelastic turns begin is interesting also, on Fig. 13-16 color marks sites in which there are such turns of crystalline lattices of grains, at various stages of strain (values of parameters correspond to experiment on fig. 9-10)
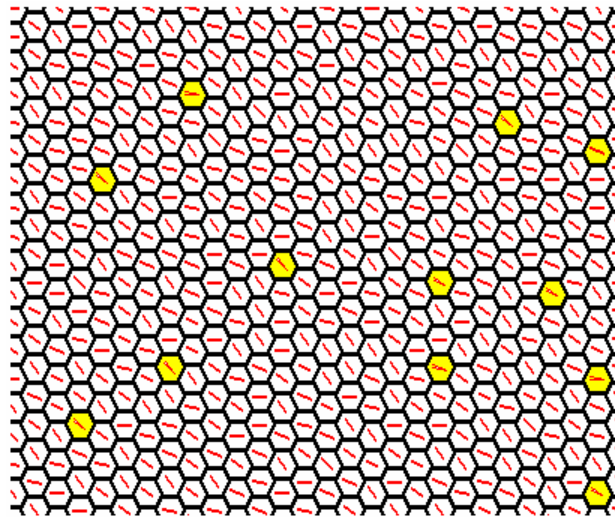

Fig. 13 the General pattern of turns of grains, at strain $\varepsilon_i = 0,05$

It is possible to note, that turns of crystalline lattices of grains begin with those grains which initially possessed the most "unprofitable" orientations, i.e. the delta circuit of which systems of slip has been canted concerning an axis of squeezing e_1 on a corner of the order $\dfrac{\pi}{6}$, thus at initial stages of a deforming it is not enough such grains, and turns in them do not give in essential change of medial value of a corner off-orientations and mean square deviation.
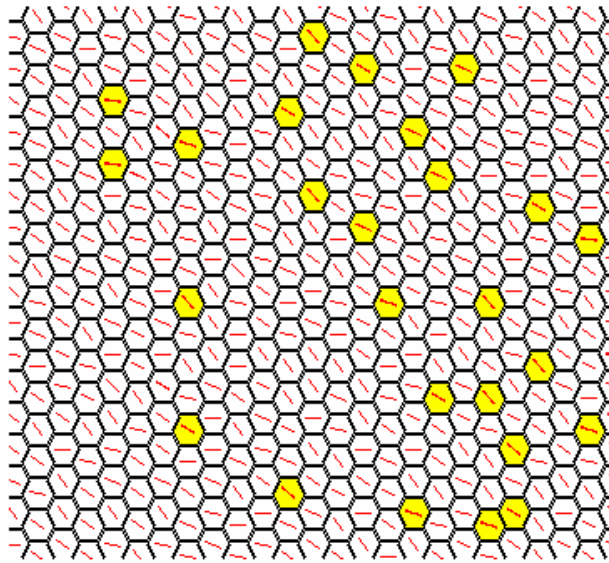
Fig. 14 the General pattern of turns of grains, at strain $\varepsilon_i = 0,1$
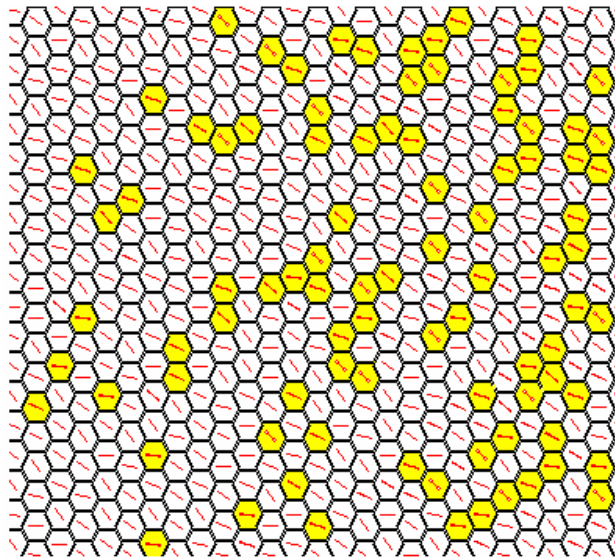

Fig. 15 the General pattern of turns of grains, at strain $\varepsilon_i = 0,25$

At increase of strains "centres" of turns start to give in the rotation motion the next grains besides enter process of turns of a grain which orientation essentially differs from $\dfrac{\pi}{6}$, and at major strains practically all grains (except for possessing) start to be developed by the best orientation plastically (fig. 16).
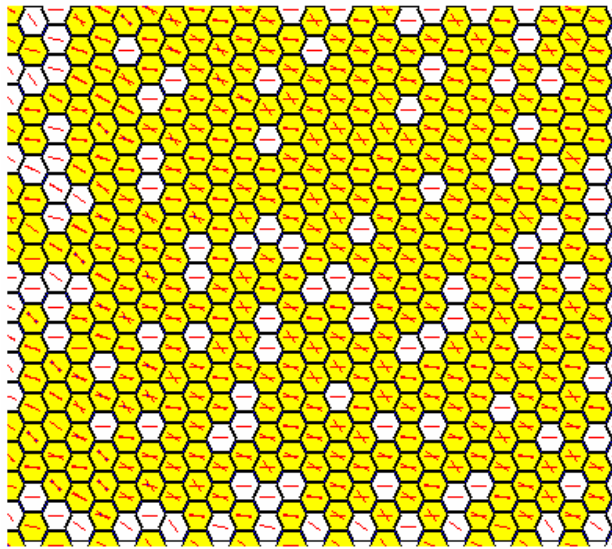
Fig. 16 the General pattern of turns of grains, at strain $\varepsilon_i = 0,45$

Besides at some values of parameters of model on a curve growth mean square deviation $D_\varphi(\varepsilon)$ is observed. This phenomenon as it is supposed, is possible to explain just process of "swing" at which grains with which gyration begins, "part forcibly" the neighbours because of what in system the degree of disorder (fig. 17) raises
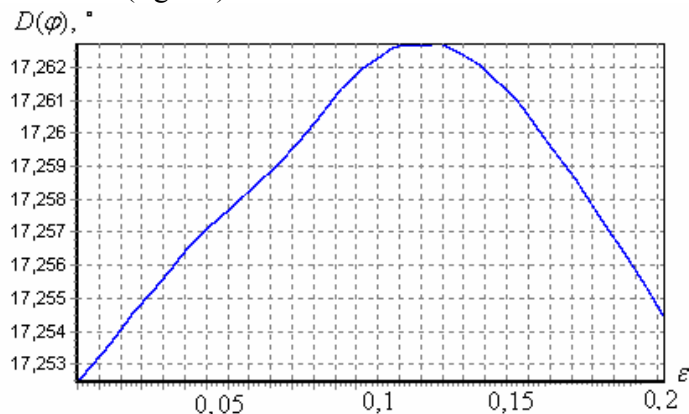

Fig. 17 Dependence mean square deviation off-orientations of grains representative volume $D(\varphi)$ from intensity of strains ε ($a = 0,35 \cdot 10^{-2}, \beta = 0,4$)

Further it is necessary to work procedure of identification of model, i.e. checkout of effects of model operation on физичность and conformity to experimental data. Unfortunately, operation on identification at the moment is not completed yet, however already now it is possible to receive some rules for rejection of the results which are not satisfying experimental data on the uniaxial loading. In particular, the literature contains the data, that дифрактометрическими by examinations set, that formation of a texture is found out at a precipitate already at 10-20 % (but not less), and formation of a texture is prolonged up to degrees of strain about 50-60 %.

Operation on search of such parameters of model at which the data received as a result of numerical experiments would well be coordinated with experimental data is at the moment carried out.

It is necessary to note as well that fact, that the results incremented with use of model, strongly differ depending on values of parameters of model α, β, and even at small changes of values of parameters results sometimes considerably differ from each other, therefore at the given stage it is impossible to speak about stability of model in relation to variations of parameters. Interesting that fact also is, that, most likely, coefficients α, β are not independent since effects, more or less compounded with experimental data, are incremented at such gangs of values α, β, that product $\alpha \cdot \beta$ has the same order.