Physical Mechanics of Materials as an Instrument to Predict and Control the Material Properties

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Abstract

To understand the real picture of the deformation of materials and to efficiently control their properties there should be uniting approaches. We developed an approach that was based upon the combination of the computer simulation with the physical experiment. Computer simulation was done using the originally designed "Cellular Model"; several new geometric objects (such as "Cloud of internal stresses", "Thick yield surface") were introduced for the in-depth understanding and predicting of the structure – properties interconnection.

Keywords: Cellular Automata, Materials, Yield Surface, Fractal

1 Introduction

Classical plastic flow models are not satisfying the modern requirements. There are two main directions in their development. The first, mathematical, is connected with the development of the general theory of rheological relationships; the second, physical, is connected with the development of the representative volume element (RVE) models which are based on specific ideas about deformation mechanisms. Within the framework of the first direction, the macroscopic experimental data is formalized; the second approach deals with the generalization of physical research results for the different scale levels that are involved in plastic deformation.

These approaches have advantages and disadvantages. In phenomenological theories, the advantages are the mathematical simplicity and laconic formulation of constitutive relations, which allows using them in practical calculations. However, the mathematical models of this class can not be considered as general, they are useful only for the description of limited range of deforming processes. On the other hand, physical theories that are based on the description of real plastic deformation mechanisms are very explanatory and predictive, but they lack mathematical simplicity.

The above circumstances lead us to the necessity of compromise that can be found in determining the constitutive relations for RVE, which structure and parameters would bear the information about microlevel and mesolevel phenomena. In this synthesis direction, the fundamental role belongs to Asaro (1983), Hill and Rice (1972), etc.

In present work, we extend the definition of such a typically "macroscopic" concept as yield surface by means of including the additional information about material structure in it. "Thick yield surface" and "cloud of internal stresses" are introduced here to fulfill this need.

Yield surface is one of the fundamental concepts of mathematical theory of plasticity (Hill, 1950). It represents a geometric image of the yield condition in the space of stresses. If a point mapping stressed condition of the material in this space resides inside the area limited by the yield surface, the material is deformed as elastic. In case when the indicated point hits on a surface, the plastic flow starts. The state mapped by points lying outside of the area limited by the yield surface is impossible. There are various interpretations concerning the form of yield surface and its evolution during the plastic deformations of material. In work by Koiter (1953) the explanation of sliding theory (Batdorf and Budiansky, 1949) is given within the framework of yield surface approach.

In several known works the yield surface is represented as the classical surface, i.e. two-dimensional object. Hypothesis of the present work is that the yield surface can be presented as thick, "foamed surface" with dimensionality exceeding two. By other words, perhaps, the yield surface is fractal, i.e. it belongs to the class of geometric objects with fractional dimensionality. Properties of such objects have been heavily studied (Mandelbrot, 1983). Apparently, fractal structure of the yield surface is determined by the fractal structure of natural materials.

In many cases, the self-similarity of objects, or "scaling" as it is used by physicists, has already allowed to take into account their structure during the macroscopic description (see, for example, Mandelbrot, 1983; De Gennes, 1979; Barrenblatt, 1979). It inspires to have new attempts, as there are evidences (see, for example, Hornbogen, 1984) about a fractal structure of metal alloys.

2 Speculations about the "thick yield surface"

Let us represent RVE (characteristic linear dimension l_{RVE}) as a structure whose deformation is determined by the deformation of its interacting elements belonging to the scale level M1 (mesolevel 1 with a characteristic linear dimension l_1). The same way we will treat M1-level elements and so on, down to the simplest elements whose deformation can be described by certain mechanisms such as sliding, sliding with the change of volume, isotropic elements with the possibility to change the volume, and so on (See Figure 1). The elements that contain sub-elements will be called complex. At any level there can be both complex and simple elements (for instance, look at the M2-level on Figure 1).

To analyze the RVE behavior and the behavior of complex elements, let us introduce the following notions:

- Cloud of Internal Stresses (ISC) - area in the stress space that represents the stressed state of an element taking into account its inhomogeneity.
- Thick Yield Surface (TYS) - area in the stress space where, in which ISC experiences a plastic strain.

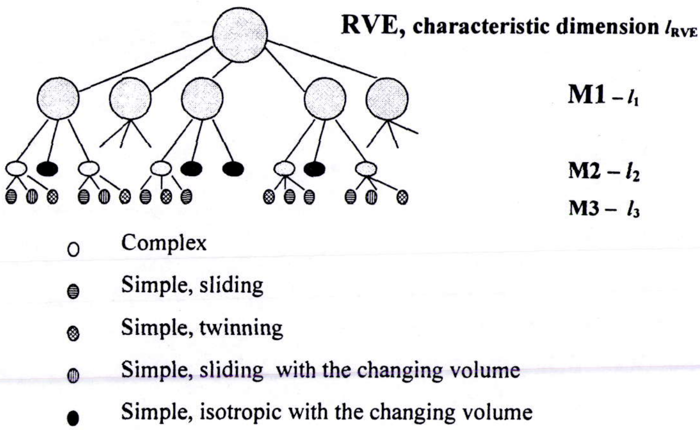


Fig. 1: Hierarchical structure of the material.

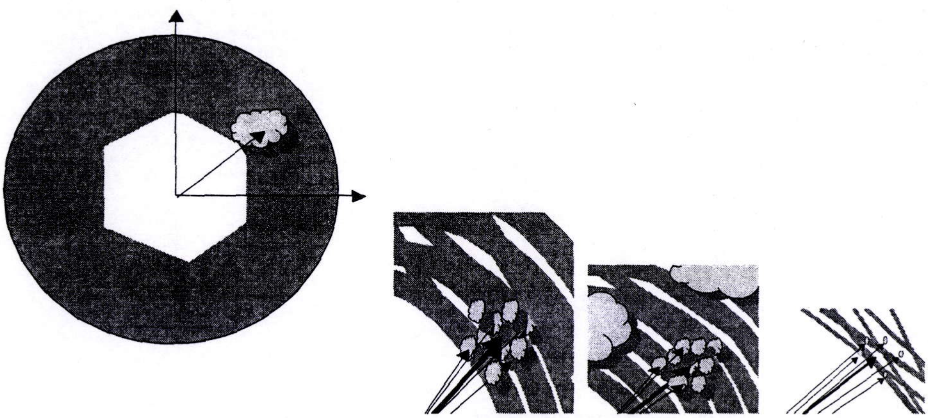


Fig. 2: Structure of ISC and TYS.

Structures of ISC and TYS are shown on Figure 2. You can clearly see that RVE recursively splits into smaller elements. Every split occurs by splitting a higher-level element into the corresponding elements of a lower level. This structure can be treated as a fractal in case of scaling.

Consider the following algorithm for constructing ISC and TYS. Initially, yield surfaces of simple elements are obtained. They are represented by thick sheets of paper on the Figure 3d. Frontal and side views of the yield surfaces of simple elements are shown schematically. In this case an element has two sliding systems, one of which can experience densification or loosening, the other one cannot. Putting these sheets together forms a book representing a complex element; book thickness is l_c. You can see

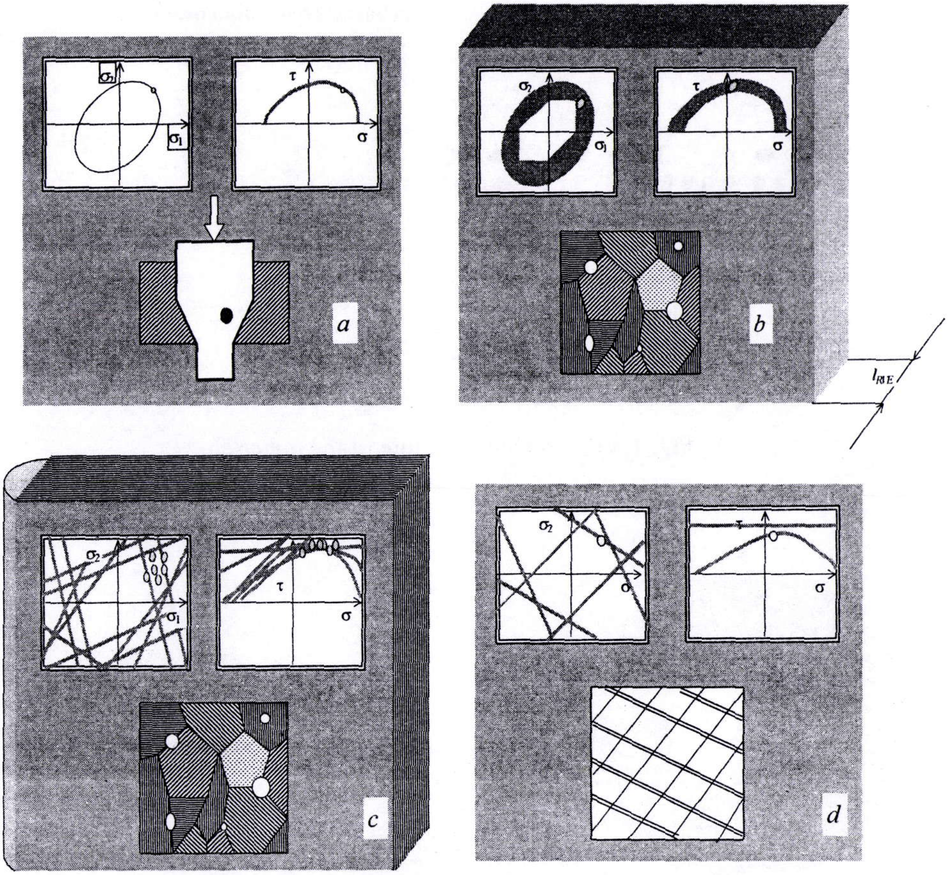


Fig. 3: Algorithm of TYS and ISC construction.
a – RVE in classical understanding; *b* – RVE as a microinhomogeneous element;
c – complex element; *d* – simple element.

TYS and ISC of the element on the cover of the book. By combining several books we can make a bigger one representing RVE; TYS and ISC of RVE are drawn on the cover of the bigger book. The last picture shows the classical yield surface of RVE, where RVE is considered to be homogeneous. That is why it appears as a sheet of paper with no thickness, and elements are shown as points in the deformed macro-body.

In order to investigate the RVE deformation and build the corresponding TYS and ISC, we developed a cellular model of inhomogeneous material that allows to predict and control the properties of materials subjected to the plastic deformation.

3 Cellular model

Structure of actual polycrystalline is simulated with the help of 3D cellular structure; the cells can be simple and complex. Simple ones do not have an inner structure; the complex cells consist of the simple and/or complicated ones while a complex cell may contain ones similar to itself, which allows to simulating of fractal structures.

In the present work, the complex cells having cubic lattice structure and consisting of 27 (3×3×3) smaller cells are considered. In general case, other spatial structures and other amounts of components can be modeled.

Neighborhood of a cell is understood as the group of its nearest neighbors. Each cell is given a coordinate (m,n,k) that defines its position (m,n,k are integers 1 through 3). Defining a boundary cell neighborhood we suppose that the cells' system is surrounded by ones similar to itself from different directions, complying with the periodical boundary conditions meaning that the neighborhood of each cell is formed by the remaining 26 cells.

Proposed model of a polycrystalline allows taking into account heterogeneity of a material at each scale level, to reflect a fractal nature of mesoscopic and structural levels and to describe easy interaction between processes happening at different scale levels.

Loaded polycrystalline is characterized by inhomogeneous stressed-strained state (SSS). To describe it we will take into consideration the stress tensor $\boldsymbol{\sigma}^{\mathbf{n}}$ and the plastic deformations tensor $\mathbf{e}_p^n$ for each cell described above. The index n in these terms specifies a level to which the considered cell belongs. The largest cell simulating the macrolevel RVE belongs to the level 1; its component 27 cells belong to the level 2; components of each from these 27 cells belong to a level 3, etc. It is obvious that there are 27^{n-1} cells at the level n.

As the plastic deformation of n level cell is stipulated by plastic deformations of its component cells of a level (n+1), we suppose

$$\mathbf{e}_p^n = \left\langle \mathbf{e}_p^{n+1} \right\rangle, \tag{1}$$

where the angular brackets mean averaging on n level cell volume.

We assume that the stress tensor and the plastic deformations tensor of n-level cell of and corresponding tensors of its n+1 level 27 cells are connected by a Kröner's relationship

$$\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^{n} = \mathbf{M} : \left(\mathbf{e}_p^n - \mathbf{e}_p^{n+1}\right), \tag{2}$$

where **M**, in common case, is the 4$^{\text{th}}$ order tensor.

The last relation shows that the difference between the plastic deformation of any (n+1)-level cell and the average value of the corresponding n-level cell produces the inner microstresses seeking to level these strains. All that leads to the redistribution of stresses within n-level cell, and then the inhomogeneous SSS arises inside the complex cells.

Relationship (1) allows calculating plastic deformation of complex cells through the plastic deformation of their components. Plastic deformation of simple cells is determined by the strain mechanism operating in them.

In particular, for plastic deformation realized by means of dislocations glide, the velocity of plastic deformation is calculated by toting components, stipulated by all systems of sliding operating in cell. In this case, for small elastic-plastic deformations the magnitude $\dot{\mathbf{e}}_p$ is calculated using the following equation

$$\dot{\mathbf{e}}_p = \frac{1}{2}\sum_{\alpha}\dot{\gamma}^{\alpha}\left(\mathbf{s}^{\alpha}\mathbf{m}^{\alpha} + \mathbf{m}^{\alpha}\mathbf{s}^{\alpha}\right), \tag{3}$$

where $\mathbf{m}^{\alpha}$ and $\mathbf{s}^{\alpha}$ are the vector normal to a sliding plane and the vector along the sliding direction in a system α, correspondingly; $\dot{\gamma}^{\alpha}$ – shear strain velocity in a system α.

The magnitude of $\dot{\gamma}^{\alpha}$ is determined by tangential stresses τ^{α} operating in a system α. The magnitude of τ^{α} is calculated in conventional way using the stress tensor of the corresponding cell:

$$\tau^{\alpha} = \mathbf{m}^{\alpha}\mathbf{s}^{\alpha} : \boldsymbol{\sigma}^{\alpha}. \tag{4}$$

The relations connecting $\dot{\gamma}^{\alpha}$ with τ^{α} for various mechanisms controlling dislocations migration could be found in a number of publications on physics of plastic deformation, in particular according to Frost and Ashby (1982)

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \exp\left(-\frac{\Delta F}{kT}\left(1-\left(\frac{\tau^{\alpha}}{\tau_c^{\alpha}}\right)^{p}\right)^{q}\right), \tag{5}$$

where ΔF is the activation energy necessary for overcoming the obstacles in lack of external stresses; τ_c^{α} – critical tangential stress for a system α; p and q - parameters depending on the mechanism controlling the dislocation migration ($0 \le p \le 1$, $1 \le q \le 2$); k – Boltsman constant; T – temperature; $\dot{\gamma}_0^{\alpha}$ – a parameter describing system α.

According to the cellular automata concept, the process of the SSS forming is researched in discrete time t_m with the discretization step Δt ($t_m = m\Delta t$, where m is the integer value). At the upper level we set the dependence of operating stress on time $\sigma^1 = \sigma^1(t_m)$. In the initial moment of time ($m=0$) we suppose that the plastic deformations $\mathbf{e}_p^n$ are equal zero at all levels.

Relation (2) will be written in a modified shape

$$\sigma^{n+1}(t_m)-\sigma^{n}(t_m)=\mathbf{M}:\left(\mathbf{e}_p^{n}(t_{m-1})-\mathbf{e}_p^{n+1}(t_{m-1})\right). \tag{6}$$

That will allow to calculate cell stresses at t_m by the plastic deformations in the previous instant t_{m-1}. Relations (1)-(6) enable one to determine the SSS of polycrystalline under the given program of the upper level loading. As the program of the deformation of material at the upper level is known, that is the tensor of full strains $\mathbf{e}^1=\mathbf{e}^1(t_m)$ is defined, the magnitude of $\sigma^1(t_m)$ is determined under the Hooke law

$$\sigma^1(t_m)=\mathbf{E}:\mathbf{e}_e^1(t_m) \tag{7}$$

in dependence on an elastic strain $\mathbf{e}_e^1(t_m)$, where $\mathbf{E}$ is the elasticity modulus tensor.

Magnitude of elastic strain is calculated under the formula

$$\mathbf{e}_e^1(t_m)=\mathbf{e}^1(t_m)-\mathbf{e}_p^1(t_{m-1}). \tag{8}$$

Relations (1)-(8) enable one to determine the polycrystalline SSS under the specific deformation program at the upper level.

Cellular model allows to study the macrobehavior of the whole ensemble of cells depending on the local microscopic laws that determine the evolution of each cell and its interaction with the closest neighborhood.

This section was intended to reveal the main structure and constitutive relationships of the Cellular Model. More explicit description of the model is given in (Beygelzimer and Spuskanyuk, 1999).

4 Evolution of the Cloud of Internal Stresses

Cellular Model was used to investigate the behavior of h.c.p. alpha-iron, results of the computer simulation of the ISC evolution inside the TYS are described below.

Figure 4 shows that each penetration of ISC in "thick yield surface" results in distortion of this set. The beginning of plastic flow of material is connected with the first signs of such a distortion. Figure 5 shows the evolution of ISC at the complex two-stage loading going in opposite directions. It is clearly seen that ISC starts to distort at the smaller outer stresses during opposite sign loading, compared to the initial loading, which reveals the Bauschinger's effect.

While the magnitude of penetration depth increases, the diameter of ISC grows, as each from the mapping points can move only along the yield plane, which corresponds to the growth of internal stresses.

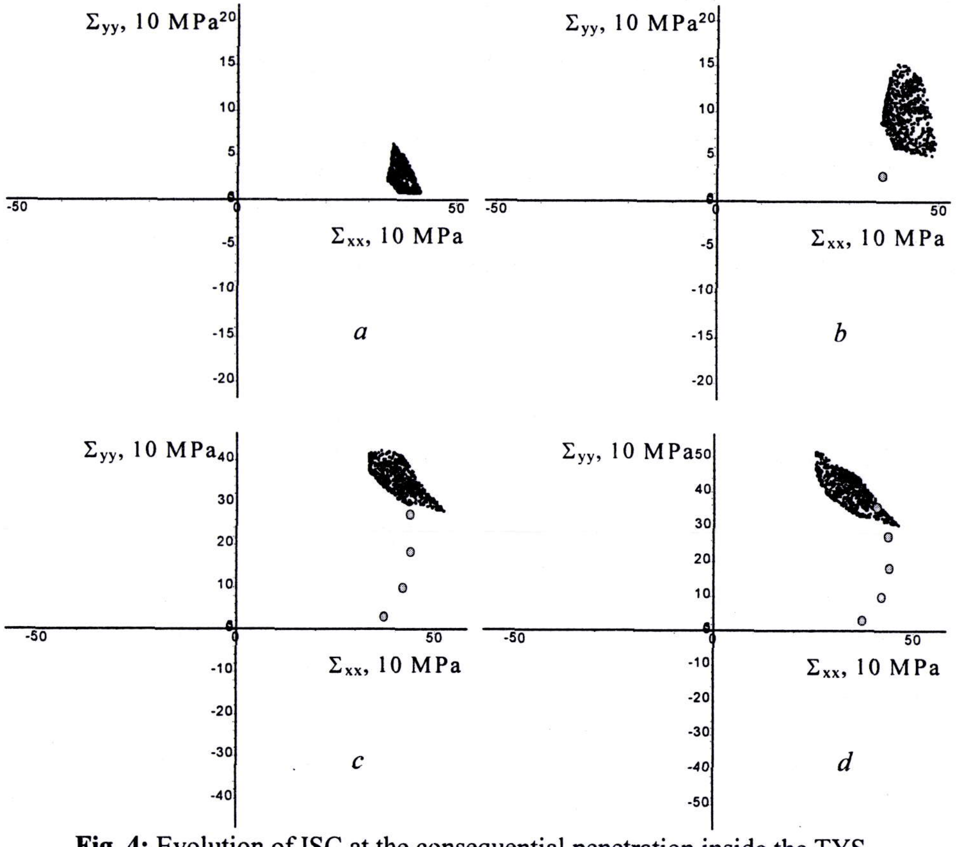


Fig. 4: Evolution of ISC at the consequential penetration inside the TYS.

The latter reaches maximum size and stops growing at the certain value of increasing strain. It means that at the rather deep penetration inside "thick yield surface" there should be rotation or fraction of yield planes, most considerably stretching ISC. Obviously, the first stated effect corresponds to the rotation of units, the second effect – to the partition of simple units, producing parts rotated one from another (fragmentation of grains). At the same time, the recess forms on the internal boundary of "thick yield surface".

Classical yield surface determines an increment of plastic deformation at each loading stage (Hill, 1950) by means of the associated flow law. It is easy to see that "thick yield surface", proposed by us, has similar properties. The difference is that in this case the macroscopic vector of plastic deformations increment of representative volume is obtained by summation of microstrain increments vectors of separate elements. Vector that is orthogonal to the appropriate yield plane determines the increment of plastic deformations, which is stipulated by a sliding system.

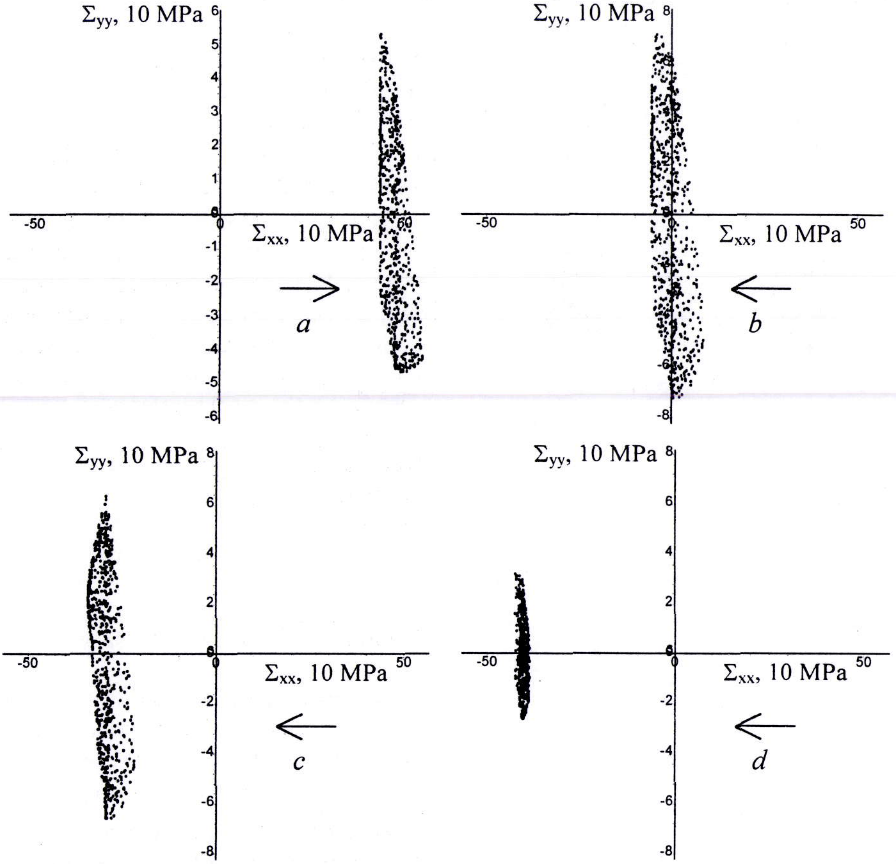


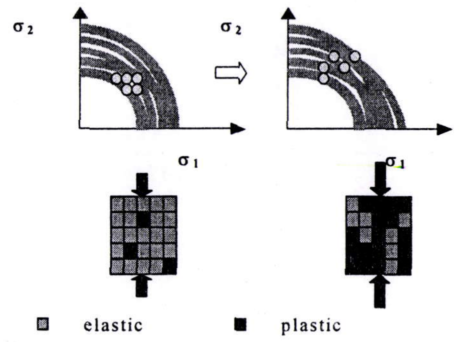
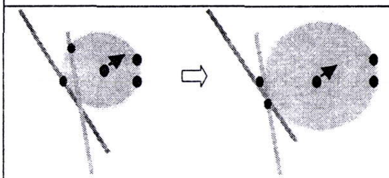
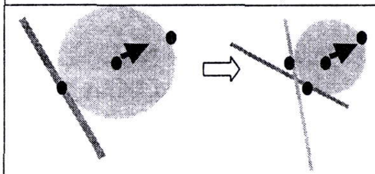
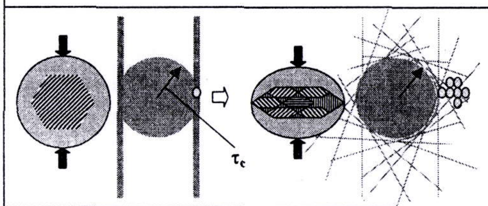
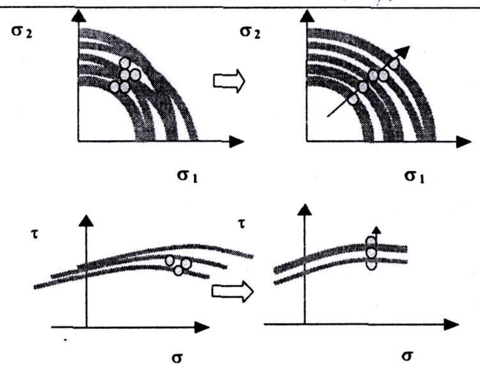
Fig. 5: Evolution of ISC at the complex two-stage loading: *a* – ISC at the end of direct loading; *b* – ISC after unloading; *c, d* – distortion of ISC at the opposite sign loading.

Velocity of polycrystalline plastic deformation growth depends on the structure of the "thick yield surface" area, occupied by ISC, and on the direction of macrostress increment vector defining evolution of ISC.

In this connection, even though the magnitude of movement into the "thick yield surface" may be identical in specific cases, there may be different increments of plastic deformation in different parts of this surface and along the different directions of movement inside it. Here, the ideal plasticity (plasticity without hardening) corresponds to some limiting formations in a "thick yield surface". To reach those, there should be indefinitely large residual strain.

In the Table 1, we will summarize our experiments with a cellular model and describe several effects of plastic deformation using the language of TYS and ISC.

Table 1: Connection of ISC evolution and TYS with the structure and macro-properties of micro-inhomogeneous materials

	**Elastically-plastic deformation and plastic flow of RVE** As load increases, more and more RVE elements become involved in the plastic deformation. In addition, ISC spreads out, and even a larger number of its components start to penetrate their yield surfaces. Plastic flow starts at the moment when the elastic cluster penetrating RVE, breaks. At this moment, a non-negligible fraction of ISC components are in their yield surfaces.
	**Hardening caused by the increase of internal stress.** Increase of ISC diameter loading the material without grain fragmentation.
	**Grain fragmentation under large deformations.** Grain fragmentation caused by large internal microstress. In addition, the diameter of ISC decreases, and partial relaxation of internal microstress takes place.
	**Hardening of RVE region caused by grain fragmentation under pressure.** "Thin" yield surface transforms into "Thick"
	**Ideal plasticity of microinhomogeneous material.** Under large plastic deformations under high pressure, the following things happen: • Material finally becomes isotropic; • TYS gains the structure of concentrically ordered cylindrical hulls; • ISC stretches along the radius of the cut of the hulls; • In addition, a stationary porosity set in the RVE.

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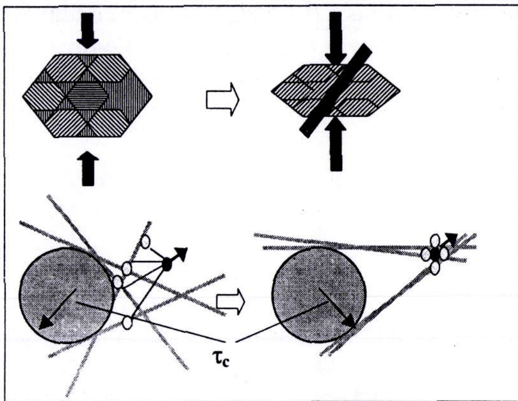
<td>
</td>
<td>Structure Formation. Loss of deformation stability with the formation of shear band
Under grain turning the following things happen:
• There emerges a corner point in TYS;
• ISC collapses to this point.</td>
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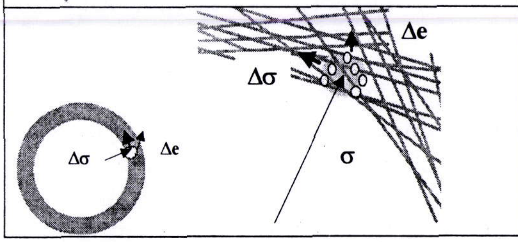
<td>
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<td>Non-proportional cyclic plasticity
Deformation under loading along TYS (Tanaka et al, 1985).</td>
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</table>

5 Conclusions

To summarize everything that was stated about the thick yield surface, it is possible to conclude that, due to a number of reasons, it is an interesting object, especially while considered together with the cloud of internal stresses. This object should not be reduced just to a new label. Several reasons from the above-mentioned are given below.

- Thick yield surface allows distinguishing between the hardening mechanisms connected with internal stresses and those connected with modifications in material structure. First ones are revealed as modifications of "cloud of internal stresses" and have no effect on thick yield surface; second ones change this surface.
- Thick yield surface allows giving a new geometric image to effects caused by internal stresses and by disproportionate loading and unloading. For example, the Bauschinger's effect is explained not as a migration of the whole yield surface, but rather as extension of the internal stresses cloud. Plastic flow during the neutral additional loading can be connected not with formation of the angular point on a smooth yield surface. Here, the center of internal stresses cloud (point mapping the stressed state of RVE as whole) is moving inside the body of thick yield surface.
- Numerical experiments show that the size and the form of internal stresses cloud depend on the trajectory and the length of path followed by the center of this cloud along the trajectory of its movement inside "thick yield surface". In turn, the geometry of internal stresses cloud and local structure of thick yield surface determine RVE deformation velocity. All this encourages to think that the geometric properties of the proposed objects can be used as parameters in constitutive relationships for RVE.

Concept of the thick yield surface allows obtaining the additional correlation between the micro-mechanical models of polycrystallines and the phenomenological theory of plasticity. Evidently, the thick yield surface is fractal. Structure of this "surface" as well as other properties of deformable polycrystalline can be investigated with the help of the developed cellular model.

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