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STRUCTURAL AND PHASE TRANSFORMATIONS IN ALLOYS UNDER THE SEVERE PLASTIC DEFORMATION

Despite the large number of works devoted to structural-phase transformations in alloys, there is still no holistic understanding of the pattern of phase transformations under the intense plastic deformation. It is probably because the plastic deformation is a complex multilevel process, in which various microscopic mechanisms operate, depending on the temperature and intensity of processing. Although the mechanisms of phase transformations have been actively discussed in recent decades, the task of classifying such transformations and identifying the main mechanisms of their implementation depending on external conditions remains urgent.

Keywords: alloys, structure, plastic deformation, transformations.

1. Introduction

Products made of fine-grained metals and alloys with high physical and mechanical properties and performance characteristics are becoming increasingly in demand in many fields of engineering and technology. The most effective and widespread technologies for manufacturing parts from this class of materials are various methods of severe plastic deformation (SPD) [1–5]. Most metals and alloys require higher processing temperatures to achieve a high degree of deformation, and experience

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significant heating during deformation. All this is accompanied by a change in the structure due to the ongoing processes of return and recrystallization. Since empirical approaches to the development of SPD methods capable to form the desired grain structure require a lot of time and money, researchers in the field of deformable solid mechanics and metal forming pay great attention to approaches and methods of mathematical modelling. Therefore, over the past few years, there has been an intensive increase in the number of publications on this topic [6–11]. The currently known models differ significantly in their approach, in the depth of penetration into the physics of the process and considered scales. This brief review is devoted to a qualitative analysis of research on the above topics and a preliminary classification of existing models by purpose, versatility and functionality. The article highlights two most common approaches to the description of changes in the grain structure during the processes of thermomechanical processing of metals and alloys: continuous (in most cases, single-level) and multilevel, based on the introduction of internal variables and physical theory. This review is devoted to publications focused on the first of the described approaches.

An overview of the results of experimental studies and existing theoretical ideas about anomalous phase transformations in alloys subjected to SPD is also given. The resulting unusual phase and the structural state determine a unique combination of physicochemical properties attractive for technological applications. Uncommon structural-phase transformations in alloys at SPD have attracted much attention over the past decades [12–18] in connection with the development of new promising materials. A common feature of a large group of transformations, which at first glance differ indeed in physical nature, is the fact that in the process of exposure, the alloy moves away from the state of thermodynamic equilibrium. It means that the mechanical energy supplied to the alloy is partially converted into the internal energy of the alloy. At the end of the exposure, the achieved nonequilibrium state of the alloy remains ‘frozen’.

In recent decades, uncommon solid-phase transformations and structural states realized in alloys during intensive exposure or subsequent heat treatment have attracted increased attention. These include disordering [19, 20] and amorphization [21, 22], reduction of oxides down to pure metals [23], formation of solid solutions in systems with negative [20] and positive enthalpy of mixing (abnormal mechanical melting) [24, 25], competitive formation and decay of solid solutions with the transition to stationary dispersed state [26, 27], dissolution of intermetallic particles [28], oxides [29], carbides [30] and nitrides [31] in steels and alloys, rapid realization of low-temperature equilibrium or metastable phases [32, 33], the formation of wide grain boundary segregations [34, 35] and grain boundary layers [36], abnormal decay with the release of nonequilibrium phases [37], cyclic reactions such as ‘amorphization–nanocrystallization’ or ‘decay–mixing’ [38]. After the cessation of exposure, the achieved state of the alloy is ‘frozen’, due to the technological attractiveness of this method of processing materials. A deep understanding of the processes developing in the conditions of SPD is of great practical importance.

It should be noted that the terms ‘grinding’ and ‘enlargement’ of grains used in the article should be understood with some degree of conditionality as referring to certain stages (most often completion) of material processing, as a result of the transformation of the grain structure in question in a particular process. Grinding in many cases is realized as the sequential nucleation of cramped embryos and their subsequent growth with the formation of a new structure. In recrystallization processes, for instance, the expansion of grains of the ‘new’ phase occurs to the absorption of grains (and reduction of their size) of the ‘old’ structure [39–44].

2. Mechanisms of Grain Grinding at SPD

An essential feature of SPD is that the sample cannot collapse during deformation, even with high degrees of deformation, and its shape remains more or less unchanged. It is especially evident when high-pressure torsion (HPT). A small disk between two anvils retains its shape regardless of the number of turns of the anvils. If, in the HPT of Nd–Fe–B alloys, the HPT withstand about 20 turns [45], then, in the case of soft alloys based on aluminium or copper, the anvil can last up to hundreds or even thousands of turns of anvils [46, 47]. In the deformation process, the number of lattice defects (vacancies, dislocations, grain boundaries) is expected to increase. However, this process does not develop at a constant rate with multiple rotations of the strikers. According to the results of direct measurements, the sample temperature during the HPT does not exceed 40 °C [48]). The rate of relaxation (annihilation) of defects increases with an increase in their concentration until a stationary state is reached at which the defect rate of formation is equal to the rate of their annihilation [49]. At the same time, the physical properties and structural parameters reach saturation in a stationary state.

Thus, when a material with a grain size of several millimetres is deformed, the grains are quickly crushed to several hundred nanometres [50] and with further deformation, their size reaches a steady value [51, 52], which depends on the SPD mode. The smallest grain size in copper and copper-based alloys, about 15 nm, is achieved by grinding in a ball mill [53]. The second most effective method of grain grinding is HPT

[54, 55]. It is followed by flat angular extrusion with channel rotation [56], equal-channel angular pressing (ECAP) [57], ECAP followed by HPT [58], ECAP followed by cold rolling [59], simple shear extrusion [60] and pressing in the defined channel [61].

As a result of SPD, a nanocrystalline (NC) state of the material is often achieved, in which the proportion of atoms located in the grain boundary region is comparable to their volume fraction. In this case, the grain size becomes an essential thermodynamic factor determining the phase composition of the alloy. The fundamental mechanism ensuring the relationship of grain size with phase composition is the formation of segregation of impurity and alloying elements at the grain boundary [62]. Segregation can significantly change the phase equilibrium of the alloy [63] and the thermal stability of the structure [64]. The role of segregation at the grain boundary is especially significant in NC alloys [65], where the proportions of atoms at the grain boundary and in the grain volume are comparable. Segregation of alloying components at grain boundaries significantly affects the strength of alloys and facilitates the transition to the nanogram state at SPD.

It is possible to distinguish several main features of structures obtained by SPD methods, which have the essential impact on the strength material characteristics.

The first feature is an increase in the density of defects in the structure and a decrease in the size of structural elements as a result of SPD. At the first stages of the formation of the ultrafine-grained (UFG) structure, with an increase in the density of dislocations in metals, a cellular structure is formed and fragmentation of the structure is observed [66.] In the same way, structure formation occurs in other single-phase f.c.c. materials [67].

At low degrees of deformation, dislocations accumulate, tangles and plexuses of dislocations form: and fragmentation of the structure is observed. The angles of disorientation between the fragments are less than 1°. As the degree of deformation increases, the size of the fragments decreases and a cellular structure is formed. With a further increase in the degree of deformation, dislocations are built into dislocation ‘walls’ and the formation of ‘knife boundaries’. These boundaries have disorientations of the order of several degrees and are very long. Opposed to the background of the developing cellular structure, microstrips, and shear bands are formed, which contributes to the formation of a grain structure. Shear bands, as a rule, are formed inside clearly defined mesofields. The microstrip formation leads to the fact that the initial grains are divided into separate sections, where various sliding systems operate [67–69]. With an increase in the degree of deformation, the angles of misorientation of grain boundaries increase and an UFG structure with smaller grain size and predominantly high-

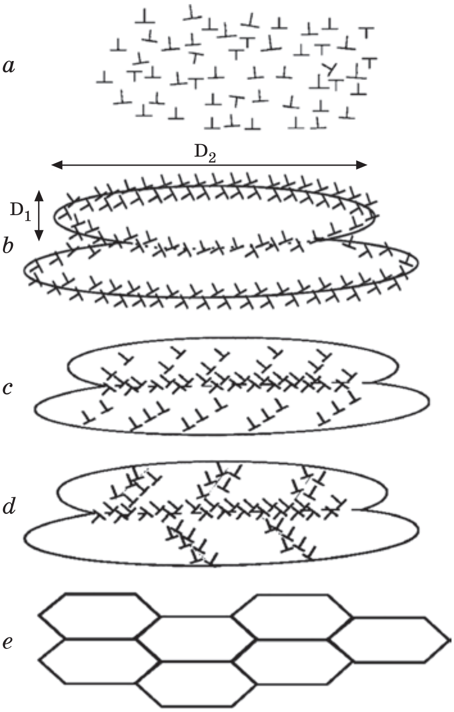

Fig. 1. Schematic illustration of microstructural evolution during severe plastic deformation. (*a*) Homogeneous distribution of dislocations; (*b*) elongated cell formation; (*c*) dislocations blocked by subgrain boundaries; (*d*) break up of elongated subgrains; and (*e*) reorientation of subgrain boundaries and formation of ultrafine grain size [69]

angle misorientation of grain boundaries is formed in the material (Fig. 1).

The second feature of the UFG structure of f.c.c. materials with low energy of packaging defects, which, in particular, include austenitic steels when deformed at relatively low temperatures or too high degrees of deformation, is the presence of deformation twins [70–72]. As the authors [73] show, the presence of twins, their shape, and the size can also influence material hardening. The size of the twins depends on the energy of the packaging defects, with its decrease, the size of the twins also decreases, reaching several nanometres [72]. As shown in Ref. [74], deformation twinning is also accompanied by the appearance of multiple secondary twins, which contributes to the formation of UFG structures. In Ref. [75], the effect of grain size on the deformation twinning process was investigated. It shows that with a decrease in the size of the initial grains, deformation twinning can be suppressed. Accordingly, in the UFG states, deformation twinning may be absent, or present to a lesser extent.

At the same time, austenitic steels are metastable and martensitic transformation is observed there when deformation is applied at low temperatures. The temperature of the martensitic transformation (MT) is determined by the chemical composition of the steel. With SPD, martensitic transformation is observed at temperatures above MT deformation martensite is formed. The formation of deformation martensite occurs by a shear mechanism [76]. The scheme of restructuring the f.c.c. grid in the b.c.c. was proposed by Bain. The theory supplemented with ideas about contractional displacements of atoms and collective rotations of microvolumes allows us to describe the restructuring of the centred cubic (CC) lattice into the b.c.c. one.

During the formation of UFG structures, the dislocation density increases significantly, respectively, and dislocation hardening also undergoes significant changes. When the dislocation density in the metal exceeds 106–108 cm^{-2}, their elastic interaction with each other begins to affect, causing braking of sliding dislocations and, as a consequence, an increase in shear stresses. The essential process of inhibition of mobile dislocations is considered to be their intersection with dislocations of the 'forest' or, in other words, with dislocations that do not lie in the primary sliding plane of the moving dislocation. As a result, dislocation clusters are formed, creating elastic stress fields that gradually lock up the sources of dislocations.

Potential barriers caused by the interaction of dislocations can be divided into long-range and short-range ones. Long-range stresses are caused by elastic stress fields of dislocations and their groups. Short-range stresses are associated with short-range forces acting at a distance of several lattice periods and arising at the intersection of dislocations, their splitting, and the formation of thresholds, kinks, and dislocation dipoles.

Wang *et al.* [77] suggested that the inhibition of a single dislocation is due to its elastic long-range interaction with dislocations forming a periodic structure in the crystal. Zeger subsequently considered the influence of groups of primary dislocations at the second stage of hardening, creating long-range stress fields. However, Zeger's theory does not consider the formation of cellular structures and plexuses of dislocations characteristic of the actual dislocation structure of deformed metals.

Adjacent to the theory of hardening by short-range stress fields are theories linking deformation hardening with the braking of the screw or mixed dislocations with the formation of thresholds on them as a result of mutual intersection. According to Gilman's theory, dislocation dipoles are formed, when dislocations with verges move, namely, stable pairs of closely spaced dislocations of the opposite sign, chains of vacancies, and interstitial atoms that hinder the movement of other dislocations.

There are two main models explaining the effect of grain size on the polycrystal flow stress. The classical theory of Hall and Petch is based on the formation of dislocation clusters at the grain boundaries. This concept explains the increase in the strength of metals with a fine-grained structure by the increased concentration of dislocations in clusters and the activation of majority sources of dislocations. The deformation-hardening model relates an increase in the flow stress during grain grinding to an increase in the dislocation density generated by the boundaries, which is inversely proportional to the grain diameter in accordance with a decrease in the free path of the dislocation. Both models give a qualitatively identical dependence of the polycrystal yield strength gain on the grain diameter, expressed by the Hall–Petch ratio.

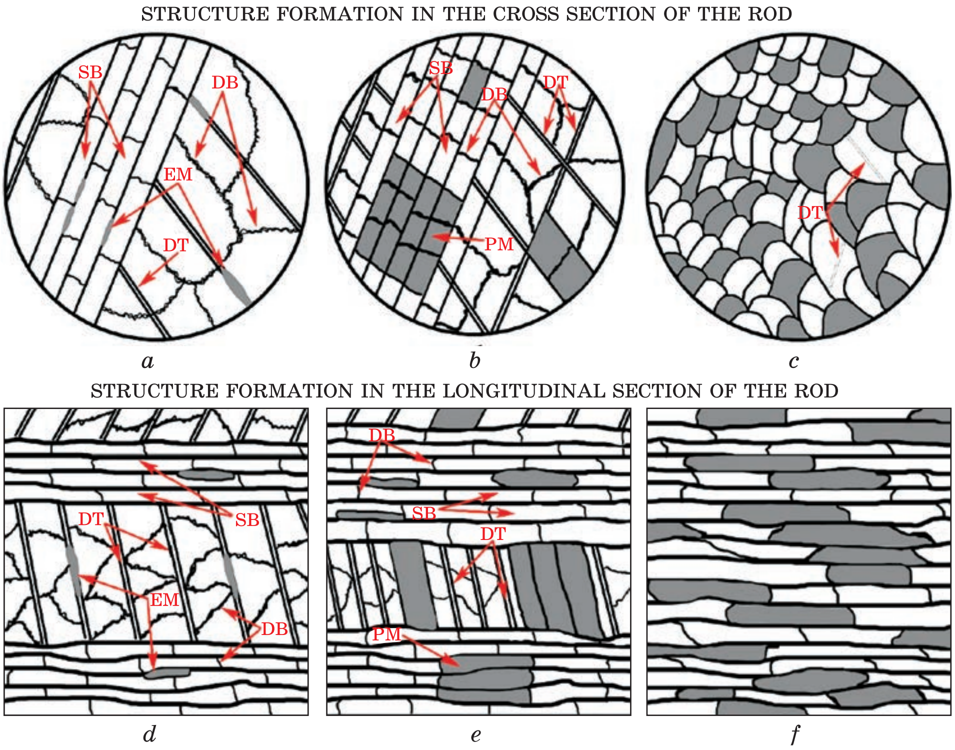

Fig. 2. (Colour online) Scheme of the 321 MASS structure formation of the rod: (*a*, *d*) first stage; (*b*, *e*) second stage; (*c*, *f*) third stage. White colour corresponds to austenite; grey colour corresponds to martensite; DB corresponds to dislocation boundary; DT corresponds to deformation twin; SB corresponds to shear band; EM corresponds to embryo of martensite; PM corresponds to packages of martensite [78]

It is shown in Ref. [78] that it is possible to distinguish clearly three stages of structure formation depending on the interval of realized degrees of deformation, which are shown in Fig. 2. The first stage of structure formation (Fig. 2, *a*) is characterized by deformation (with degrees up to $e = 0.56$) in accordance with the twinning mechanism, *i.e.*, the TWIP effect that forms a barrier for dislocation sliding with the formation of dislocation cells. Deformation twins cross the boundaries of previously formed dislocation cells and then act as barriers to dislocation movement that causes the formation of cells inside microvolumes bounded by deformation twins. Inside austenitic grains, twinning occurs mainly in one system. Twins in steels with a face-centred cubic lattice are formed due to radiation from a partial Shockley dislocation in a system of planes {111}. In addition to the deformation twins, the structure includes formed shear bands that split austenitic grains into microvolumes of austenite with a lamellar structure oriented in a predictable way along the axis of the rod (Fig. 2, *d*). Additionally, at such degrees

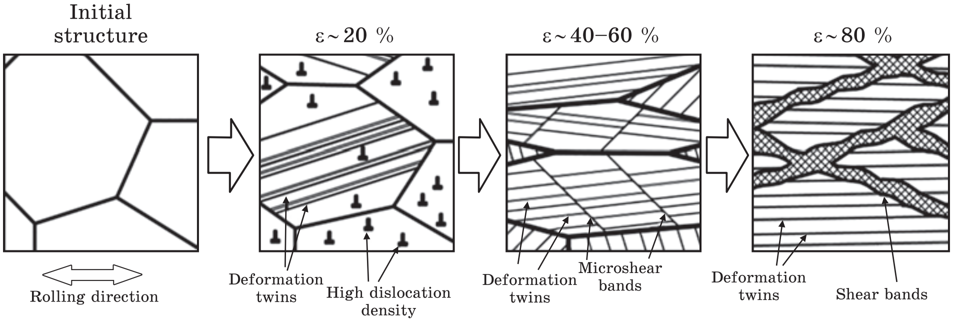

Fig. 3. Scheme of microstructure evolution during cold rolling of the Fe–23Mn–0.3C–1.5Al steel [79]

of deformation, martensite nuclei are formed in the structure caused by deformation. Thus, at the first stage of deformation, a lamellar austenitic structure with deformation twins and shear bands is formed.

At the second stage of structure formation (the degree of deformation in the range from $e = 1.00–1.71$), the process of deformation-induced twinning on secondary systems increases, which leads to the transformation of the lamellar structure obtained at the first stage into a block trapezoidal structure in cross section. However, this provides the basis for martensitic transformation caused by deformation due to the formation and growth of embryos with further formation of martensitic packages.

Thus, at this stage, a block trapezoidal austenitic-martensitic structure is mainly formed (Fig. 2, *b*) in the transverse direction in combination with obtaining a ribbon structure in the longitudinal section (Fig. 2, *e*).

At the third stage, in most of the studied fields of the cross-section microstructure of the rod, the block trapezoidal structure is transformed into an equiaxially granular one (Fig. 2, *c*), which is probably caused by the rotation of each part until an equilibrium orientation is reached. In addition, deformation twins are not found in most grains, except for the largest grains, that is due to the so-called restriction effect. In the longitudinal section at this stage, a ribbon austenitic–martensitic structure is formed (Fig. 2, *f*), that is further fragmented by dislocation and interfacial boundaries in the transverse direction.

The paper [79] shows the effect of cold rolling on the microstructure and mechanical properties of TWIP steel. Extensive deformation twinning occurred during rolling. Figure 3 shows a diagram describing the evolution of the microstructure during deformation. Three well-defined stages of microstructural evolution can be distinguished. At stage I, rapid hardening is associated with a sharp increase in dislocation density and single twinning within individual grains. At stage II, extensive multiple twinning occurs in the compression range of 20–40% and the quantity of lattice dislocations remains unchanged. The insides of the initial grains are divided into nanoscale crystallites of rectangular shape, separated by the boundaries of the twins. At stage III, during further rolling, the evolution of microdrive bands occurs simultaneously with multiple twinning, creating a hierarchy of grain-boundary aggregates. Microscale crystallites bounded by the borders of the shear bands are subdivided into nanoscale crystallites, bounded by the borders of the twins.

A series of articles [80, 81] is devoted to the construction of a dislocation-disclosure model to describe the grinding of a grain structure. The grinding of grains is considered as a result of the formation of a block-cellular structure due to the formation of nuclei of cell boundaries and the 'capture' of dislocations by them, the formation of clusters of dislocations and shear bands, the formation and movement of disclinations. With continued plastic deformation, reversals along the boundaries of cells and blocks of cells increase, and the angles of rotation along the boundaries of blocks increase with higher speed. The description of block boundaries is carried out using the concept of partial disclosure dipoles. A model is proposed to describe the microstructure, including evolutionary equations for dislocation densities, partial mobile and immobile disclinations, cell sizes and cell blocks, and angles of disorientation of cell blocks. Using the model, the processes of grain grinding for different orientations to the characteristic directions of deformation of samples from various metals and alloys are considered. To implement the developed model and its modifications, it is proposed to use the Taylor approach. A decent correspondence of theoretical results to experimental data is shown.

In the analysis [81], the mechanism of restructuring the grain structure in ultrafine-grained and nanocrystalline materials is considered due to the movement of grain boundaries under the action of applied stresses. The boundaries are represented by sections of planes, along which the disorientation of the adjacent crystallites takes place; a discretionary approach is used for the description. Based on the energy consideration, various variants of the reciprocal movement of grain boundaries in a flat formulation acceptable for the study of thin films or coatings are analysed. It is noted that borders can move towards each other or move away from one another, unite, or split into two new boundaries (with different disorientation angles). Examples of the application of the proposed approach for determining the limit values of grain sizes in the SPD of copper and nickel samples are given. Among the deformation mechanisms, the movement of grain boundaries under stress is of particular interest (Fig. 4), since it promotes both plastic flow and grain growth in nanomaterials, as well as in their coarse-

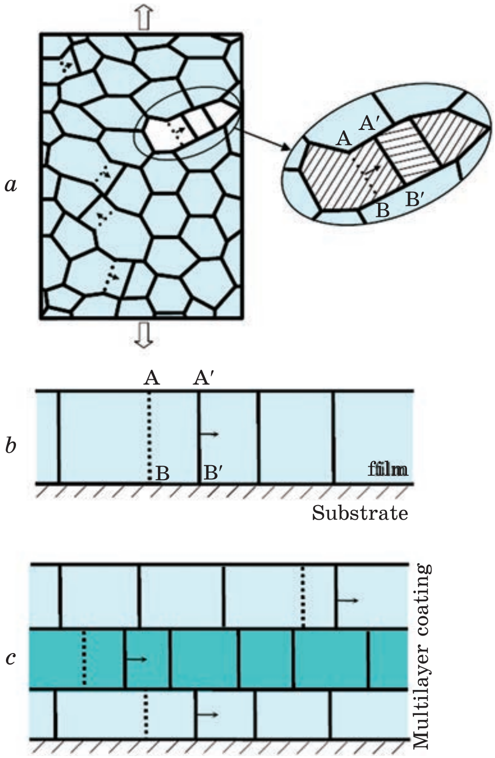

Fig. 4. Stress-driven GB migration in (*a*) nanostructured bulk material, (*b*) film with nanoscale or ultrafine grains, (*c*) multilayered film with nanoscale or ultrafine grains (schematically) [81]

grained analogues. That is the movement of grain boundaries under stress not only leads to plastic deformation of nanomaterials but it is also capable of causing pronounced changes in the grain structure, which controls the outstanding mechanical and functional properties of these nanomaterials.

In Ref. [82], the main mechanisms of meso- and microstructure changes during hot deformation of samples from AA5052 and AA7050 alloys are considered, which include: the generation of dislocations; formation of subgrains due to the formation of dislocation walls; migration of small-angle boundaries, accompanied by rotation of subgrains and transformation of boundaries into large-angle boundaries; migration of large-angle boundaries with the absorption of dislocations, small-angle and parts of the large-angle boundaries, the formation of new grains (continuous dynamic recrystallization). A system of equations is given to describe the action of these mechanisms, most of which are modifications of previously known phenomenological relations. The results of macro experiments (for torsion and precipitation at different temperatures and deformation rates) were used to identify and verify the model as a whole. A comparison of theoretical and experimental data on several parameters (the dependence of the flow stress on deformation, the proportion of large-angle boundaries, and the evolution of the average grain size) demonstrates a decent correspondence.

Figure 5 shows the above mechanisms contributing to the evolution of the microstructure and viscoplastic flow of aluminium alloy during hot stamping: (*1*) accumulation of dislocations during moulding (Fig. 5, *a*), which lead to the formation of new subgrains with small-angle grain boundaries (Fig. 5, *b*); (*2*) migration and accumulation of dislocations of the same sign in the grains with small-angle boundaries and subsequent

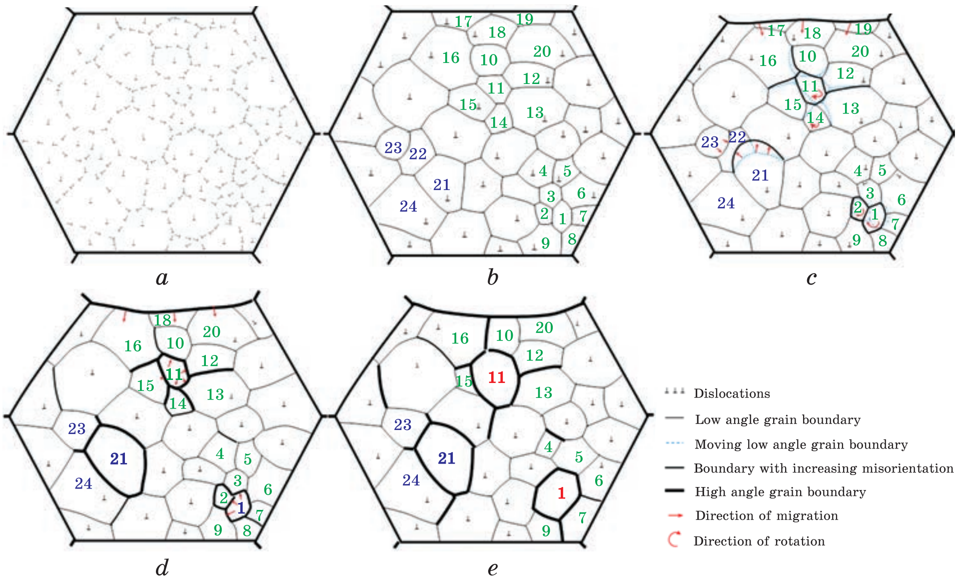

Fig. 5. Schematic illustration of microstructural evolution during deformation. Here, (*a*) dislocation accumulation, (*b*) formation of the low angle grain boundaries (LABs) and subgrains, (*c*) increase of LABs misorientation due to subgrain rotation and LABs migration, and reduction of LABs due to the high angle grain boundaries (HABs) and LABs migration, (*d*) formation of HABs from LABs, (*e*) reduction of LABs and HABs due to HABs migration [82]

shifting of grain boundaries, which leads to rotation of the subgrains, *e.g.*, subgrains *1*, *2*, *4*, *11*, and *14* in Fig. 5, *c*; (*3*) rotation of the subgrains leads to an increase in the misorientation angle and eventually transforms part of the small-angle boundaries into large-angle ones, *e.g.*, subgrain *11* in Fig. 5, *b*, *c*, *d*); (*4*) migration of small-angle boundaries absorbs grain dislocations and leads to an increase in misorientation, gradually turning part of the small-angle boundaries into large-angle ones, for example, small-angle subgrains *21* in Fig. 5, *b*, *c* in large-angle grains *21* in Fig. 5, *d*; (*5*) migration of large-angle borders sweeps away part of the larger and small-angle borders, which leads to a decrease in the corresponding areas. For example, migration of the initial large-angle grain boundary leads to the annihilation of the small-angle boundary surrounding the subgrains *17* and *19* from Fig. 5, *c* to 5, *d*; movement of newly formed large-angle boundaries leads to the annihilation of small-angle ones surrounding the subgrain *3* from Fig. 5, *d* to 5, *e*. Movement of grains with large-angle boundaries sweeps away part of the grains with small and large-angle boundaries that surround grain *11* from Fig. 5, *d* to 5, *e* [82].

In Ref. [83], a slightly different view of the development of fragmentation is proposed, which is based on the regularities of the forma-

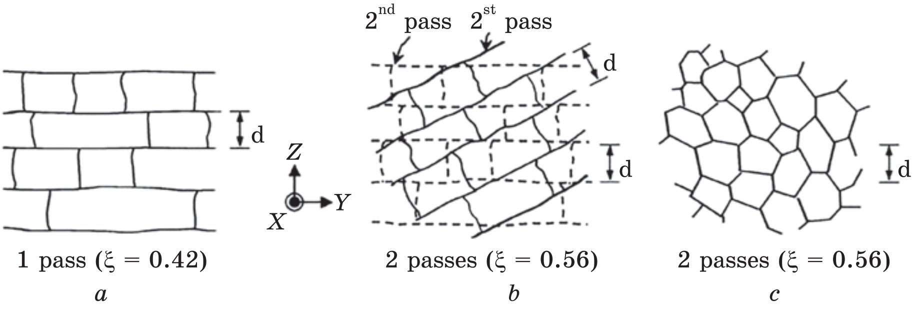

Fig. 6. Microstructural model showing grain refinement after pressing through *1*, *2*, and *4* passes: the parameter ξ denotes the fraction of high-angle boundaries [83]

tion of band structures. The mechanisms of the formation of shear bands, the orientation of the boundaries of which differs from the orientations of the planes of light sliding, have not yet been fully elucidated. I have not found a scientific explanation for the fact of alternating changes in the sign of the angle of disorientation of the crystal planes of neighbouring bands. The authors [83] proposed a model for the nanostructure formation during deformation by equal-channel angular pressing (Fig. 6). However, the question of the reorientation-bands' formation mechanism was not discussed in this work.

An fascinating interpretation of the shear bands is given in Ref. [84], where, based on the consideration of the joint action of two sliding systems, it is suggested that the shear band begins at the intersection of the two sliding systems, in other words, a stress mesoconcentrator arises, called 'christon', *i.e.*, the carrier of lattice displacement quanta during shear deformation. Such a concentrator is able to polarize actively the medium at mesoscales, creating an excessive dislocation charge of the opposite sign in the vicinity of the initial concentrator, forming a dipole pair with the initial charge.

The conclusions made in Ref. [85] are largely consonant with the ideas about the formation of boundaries with discrete misorientation of mating regions in terms of the formation of dipole dislocation charges (described earlier in this section when discussing the bending mode of deformation). In the case, when the dislocation dipole has a configuration of two flat dislocation clusters of different signs, the displacement field around such a charge represents a cylindrical bend (similar to the curvature of a tile).

Consequently, it can be imagined that during deformation, a periodic elastic displacement field arises, which, under certain conditions, can relax into shear bands with alternating changes in orientation and non-crystallographic direction of the boundaries.

When the sample enters the matrix, it appears in the field of increasing gradient stresses. Nevertheless, in addition, additional stresses arise in the material associated with the need to reorient the lattice to a favourable location of the planes of light sliding relative to the direction of external influence. This process causes the formation of dipole dislocation charges and the subsequent wave field of displacements of atoms forming the bending of crystal planes.

The nature of fragmentation consists in the deformation grinding of the structure, which consists in splitting the initial grains into smaller disoriented areas separated by small-angle and medium-angle boundaries. At the same time, the misorientation angles θ increase with the growth of deformation according to the linear law. In the works of V.V. Rybin, it was determined that at temperatures below the recrystallization temperature, fragmentation patterns are universal and persist under any deformation methods for structural metals of any chemical composition, crystal structure and initial structure [86]. During fragmentation, the dislocation structure evolves (during plastic deformation) the steps following below:

(i) increasing the density of uniformly distributed dislocations to 10^{12} m^{-2};

(ii) redistribution of dislocations (tangles, plexuses, *etc.*) and their annihilation (the density increases to 10^{14} m^{-2});

(iii) formation of a poorly oriented cellular structure separated by imperfect dislocation boundaries;

(iv) the emergence of collective forms of movement of strong dislocations, the appearance of plastic reversals of one part of the crystal relative to the other.

In a deformed metal, with an increase in the degree of deformation, the quantity of defects increases. When the possibility of uncorrelated movement of individual dislocations is exhausted, the collective migration of interacting dislocations occurs due to the occurrence of rotational plasticity modes. At the first stages of fragmentation, fragments are formed in the structure, disoriented at small angles, with a developed substructure inside, as the deformation continues, the disorientation angles increase. The final stage of fragmentation is the formation of isotropic fragments, disoriented by large-angle boundaries and practically free from dislocations.

In essence, fragmentation is the result of plastic accommodation, heterogeneity of structural defects evolves into a fragmented substructure consisting of dislocation subboundaries of deformation origin and an internal space containing or not containing dislocations. To date, fragmentation processes have been well studied on austenitic steels, in titanium and aluminium, as well as in ferritic steels during cold deformation.

The article [87] is devoted to the theoretical and experimental study of grinding for various SPD processes (ECAP, torsion at high hydrostatic pressure, orthogonal cutting). The experimental results show that in all the processes studied there are some limits to grain grinding. A strength approach was used for theoretical research. It is assumed that the applied mechanical work is spent on increasing the energy of the defective microstructure (dislocations, vacancies; when constructing the model, this contribution is neglected), a change in the surface energy of the grains, and an increase in temperature. It is assumed that grain sizes change due to two competing processes: grinding due to deformation (possible at room temperature) and growth due to thermally activated diffusion, a simple evolutionary relation is proposed to describe the change in grain size (an ordinary differential equation). When determining the temperature change, both adiabatic conditions and the possibility of heat energy runoff due to heat transfer to the environment are considered. The results of calculations of the change in the average grain size for aluminium, copper, and nickel samples subjected to the specified SPD processes are presented.

Particular attention, when we consider the grain grinding processes, is paid to the consideration of disclinations and their interaction with dislocation ensembles [86]. The research results indicate the emergence of ‘new’ structures in the depths of the ‘old’ and the gradual absorption of the latter by the former. In particular, the grinding of the grain structure begins with the formation of dislocation and disclosure walls, which cause the turns of parts of the crystallites relative to each other; the ongoing plastic deformation leads to an increase in the disorientation of crystallites, the formation of subgrains and new grains smaller than the original sizes. Based on the obtained data on the evolving microstructure, numerous so-called ‘physically oriented’ models are based, a significant part of which operates with continuous variables to describe the interacting dislocation and disclosure substructures changing during deformation [88–92] of the process is the presence of an assertive effect of metal hardening under the combined influence of plastic deformation and temperature. The changes in the structure of steel caused by riveting are usually stable and persist after double-phase recrystallization $\alpha\to\gamma\to\alpha$, therefore, preliminary plastic deformation can play a significant role in the formation of the austenite structure during subsequent heat treatment. The acquisition of properties is affected by the hereditary transmission of structural defects: the density of imperfections, fragmentation of the structure, as well as the grinding of austenitic grains.

The nature of the physical processes occurring at the A7075 alloy KVD varies depending on the deformation mode. The predominant mechanism of relaxation of internal stresses in a wide range of true deformations $e \le 6.4$ is fragmentation, while the structure is crushed to the nanoscale. The average grain size at $e = 6.4$ is 55 nm. At $e \ge 6.9$, another channel of elastic energy dissipation begins to operate in the alloy, namely, low-temperature dynamic recrystallization. In this case, less defective grains with clear boundaries appear in a varied structure consisting mainly of fragmented grains [93].

It is established that the change of one type of structure to another in the A7075 alloy occurs against the background of two-phase transformations induced by plastic deformation and competing with each other: deformation dissolution of dispersoids of refractory metal aluminides and the $MnZn_2$ phase ($4.1 < e < 4.8$) and deformation kinetic aging with the release of a metastable hardening n'-phase (> 5.5). Thus, the transition from a fragmented structure to a recrystallized structure occurs through an additional channel of relaxation of elastic energy, namely, phase transformations. Summing up the experiments carried out, it can be considered established that in the process of torsion under high pressure at high degrees of deformation ($e = 5.5$–6.4), a nanostructured state is achieved in the A7075 alloy. All the characteristics of such a structure described above indicate that it is formed by fragmentation of subgrains, in other words, due to the bending of the crystal lattice and rotational modes of deformation [93].

The bending of the crystal lattice is carried out because of the development of crystallographic sliding of lattice dislocations, and rotational modes of deformation are realized using grain boundary slippage caused by the movement of partial disclinations. The same mechanism of the elastic-energy relaxation supplied from the outside was observed in this alloy and the process of its high-speed deformation by the DCAP method. The transition to another mechanism of elastic energy relaxation, dynamic recrystallization, is realized in the studied alloy only at an extensive amount of accumulated deformation ($e = 6.9$), achieved with HPT [93].

3. Continuous Models of the Grain Structure Grinding

A brief overview of the results of experimental studies and the main physical mechanisms of grinding is given in Ref. [94], which mainly considers studies of SPD at low temperatures, obviously lower temperatures, at which the recrystallization process becomes significant, and solid-state phase transitions can be realized. Our article is devoted to the review of existing continuum models focused mainly on the description of changes in the grain structure under these conditions [95].

At the same time, the mentioned transformations can occur in metals and alloys in the SPD processes even at temperatures significantly different from the characteristic ranges of their realization under the action of only thermal factors. Due to the complexity of separating the various mechanisms, changes in the grain structure of the work, in which the latter are the result of the implementation of several mechanisms, will also be reflected in the review.

A significant part of researchers considers the accumulation of excess internal energy in the material due to the generation of crystal lattice defects as the main reason for the change in the grain structure. In the mechanics of a deformable solid, accumulated inelastic deformations are usually used to assess the level of 'defect', the measure of which is the integral over the processing time of the intensity of the plastic (viscoplastic) component of the velocity strain tensor. It should be noted that this measure does not have a clear physical meaning (expressed through the characteristics of the main mechanisms of inelastic deformation at the meso- and microlevels) [96]. The 'transparent' mechanical (geometric) meaning of this measure is only for the easiest loading of a macroform by uniaxial tension–compression; in this case, it is equal to the longitudinal logarithmic deformation.

In addition, it is known that the behaviour of mono and polycrystalline metals and alloys, the evolution of their defective structure at both macro- and meso- and microlevels is significantly influenced by the type of stress–strain state, the complexity of the loading process.

The internal energy accumulated during inelastic deformation relaxes because of the activation of physical mechanisms of various structural-scale levels, the intensity of which depends on the ranges of parameter values describing the thermomechanical effects acting on the material under study. Relaxation of internal energy is accompanied, as a rule, by a significant restructuring of the micro- and mesostructure (including grain and dislocation structures). At relatively low deformation temperatures, the structure restructuring is carried out mainly due to mechanical influences. Under these conditions, intensive multiplication of dislocations, their interaction with each other, and self-organization lead to the formation of cellular, block-cellular, fragmented structures, reversals of fragments and subgrains relative to each other [86, 97] and eventually to a crushed 'new' grain structure.

To describe these mechanisms within the framework of phenomenological theories, models formulated in terms of mechanical variables (stresses, inelastic deformations, strain gradients) are used, sometimes with the introduction of internal variables. With an increase in the processing temperature, the mechanisms caused by diffusion (atoms, vacancies, *etc.*) are activated, due to which return and recrystallization are realized, also leading to a change in the subgrain and grain structure.

From a geometric (kinematic) point of view, the change in the grain structure is associated with the reversals of individual parts of the grains relative to each other; when a certain value (usually 15°) is reached, the disorientation of the grain subdomains relative to the orientation of the 'mother' phase and neighbouring parts, these subdomains are considered separate grains. The models, in which along with translational degrees of freedom for material particles, rotational modes of motion are also introduced, appeared in continuum mechanics (primarily for elastic materials) back in the early twentieth century [98].

Two different scenarios of the evolution of the grain structure in the SPD processes, which can be superimposed on the mechanism of crystallite grinding, are considered from the energy standpoint in [99, 100]. A common feature of the considered scenarios is their cycling. According to the first of them, the process of crushing (primary fragmentation) is replaced by primary recrystallization, followed by secondary fragmentation, after which comes the stage of dynamic recrystallization, and so on. In the second scenario, after the primary fragmentation stage alternating, processes of amorphization and nanocrystallization follow. The authors note that the 'trajectory' of structural rearrangements is determined by such factors as the temperature, the size of the dislocation Peierls barrier and their ability to diffuse rearrangements, and the energy difference of the crystalline and amorphous states. The evolution of the defect structure (point defects, dislocations), their interaction, restructuring, and the formation of new boundaries are considered the driving force of the processes of crystallite change.

The transition to fragmentation and amorphization (for some materials and/or deformation modes, to a solid-state phase transition) occurs after the possibility of relaxation of the supplied mechanical energy is exhausted due to dislocation mechanisms and point defect flows. Grain sizes do not explicitly appear in the proposed model. Another characteristic is introduced to describe the grinding process, *i.e.*, the density of the boundaries.

It is proposed to use a qualitative model based on the application of the first principle of thermodynamics (the law of conservation of energy) and the Landau theory of phase transitions to describe the processes of SPD. By this, the terms responsible for the intensity of various types of defects are introduced into the expression of internal energy along with elastic strength dissipated on plastic deformations and thermal (coming from outside the system) energies. At the same time, the essential type of defect is considered to be high-angle grain boundaries, the formation of which determines the grinding of grains; the density of borders is taken as a quantitative measure of this type of defect.

The article [101], mainly devoted to the review of the results of experimental studies of the mechanical behaviour of single-phase polycrystals at creep at elevated (in the vicinity of 0.5 homologous) temperatures, also discusses the formation and evolution of the subgrain structure. The subgrains begin to form at a transitional stage, and at the phase of steady creep, they form a stable and homogeneous system. It is pointed out that the determining role for the formation of the subgrain structure of reproduction and self-organization of dislocations forming flat clusters and walls, which are further transformed into the boundaries of the subgrains. The latter has high mobility, which determines the growth processes of the characteristic sizes of the subgrains.

Further, the point of view of Yu.M. Vainblat and the VILS employees [102, 103] on the processes occurring in the alloys of the Al–Mg system is presented. The formation of deformation textures in aluminium alloys is described as follows. At both high and low temperatures, the elementary mechanism of deformation of aluminium and its alloys is a shift along the plane {111} in the direction ⟨110⟩. Sliding begins in the most favourably oriented grains, and then, as the stress increases, it spreads to all other grains. Shear deformation is accompanied by a regular rotation of the crystal lattice relative to external forces. In addition, each grain is affected by neighbouring grains, forcing it to change its shape by the deformation scheme of the entire product or part of it. As a result of co-ordinated turns with a degree of deformation of 30–50%, the grains acquire final orientations, which do not change or change slightly with further deformation. The nature of the last position depends on the deformation scheme. Due to the symmetry of the deformation process, grains can take with equal probability one of several orientations symmetrical concerning the main directions of deformation. The texture is usually described using these preferential orientations, otherwise called texture components.

The microstructure of the deformed semi-finished product is formed because of two processes: the gradual transformation of the original microstructure and the creation of new microstructure elements of deformation origin. The first process consists in changing the shape of the grains by the deformation scheme in a given cross-section zone, and the second is the formation of new grain boundaries. There is a definition of grain as an area surrounded by a high-angle boundary (in other words, a boundary with a misorientation angle of more than 10–15°) and containing no such borders within itself. In cast metal, dendrite meets this definition. The proof that new boundaries arise during deformation experiments on pressing and rolling single crystals, as a result of which they turned into polycrystals. The degree of hereditary influence of the original structure is weaker, the more the process of formation of new boundaries is developed. New boundaries are formed in cases, when it is problematic to transform the initial shape of the grains into the final one and when there is a distinct texture in the work piece that is very different from the structure of semi-finished products. Accelerated formation of new boundaries is observed, for example, during the deformation of cast grains having a complex shape and with longitudinal precipitation of the pressed billet. In the latter case, both factors are undertaken, since the texture of the pressing is very different from the texture of the precipitation.

If the grain elongation directions coincide during the first and second deformation (double pressing, rolling without edging), then, new boundaries almost do not arise and new grain sizes are easy to calculate, knowing the old dimensions, scheme, and degree of deformation. It is also unlikely that new boundaries will form when the grains in the work piece are equiaxed, and there is no distinct texture (recrystallized work piece).

4. Phase Transformations in SPD

Phase transformations can include both the phenomena of phase dissolution, oxidization, and other chemical transformations, as well as phase transitions in the solid state, for example, thermoelastic martensitic transformations discovered by G.V. Kurdyumov and L.G. Khandros in 1949. Therefore, phase transformations in alloys include several physically different phenomena that lead to changes in the physicochemical characteristics of the material: (a) changes in the crystal structure as a result of lattice shifts, without changing the chemical composition and without the participation of diffusion processes (allotropic and martensitic transformations); (b) loss of ordered phases and disordering, requiring migration of atoms over distances of the order of the lattice parameter; (c) transformations with a change in chemical composition (decay and formation of a solid solution), requiring diffusion processes.

Many authors note that with intensive mechanical action on the substance more complex transformations can be occurred. In this way, a chain of cyclically alternating transformations in the Ti–Co system was recorded in Ref. [104], and the transformation that began tended to complete with an increase in temperature after the termination of mechanical activation.

A complex chain of transformations:

$$\beta\text{-FeB} \rightarrow \alpha\text{-FeB} \rightarrow \beta\text{-FeB} + \alpha\text{-FeB} \rightarrow \beta\text{-FeB} + \mathrm{Fe_2B} +$$
$$+ \text{amorphous phase} + \mathrm{B} \rightarrow \alpha\text{-FeB} + (\mathrm{Fe_2B})^* + \text{amorphous phase} + \mathrm{B}$$

with possible cycling was observed in Ref. [105].

Atomic disordering was observed in intermetallic compounds after SPD. In $\mathrm{Ni_3Al}$, after intense torsion deformation with a pressure of $P = 8$ GPa, a complete disordering of the atomic structure was recorded by x-ray diffraction analysis. However, when heated at 3500, a partial restoration of the long-range order was observed. A similar treatment of TiAl intermetallic also led to disordering [106].

Parallels are often drawn between the decay of alloys during plastic deformation and the formation of segregation on the sample surface during irradiation. It is due to a combination of experimental facts, according to which the phase transformations under plastic deformation usually develop in the region of boundaries and triple joints of grains. Theoretical concepts according to which the sample under plastic deformation is an open energy system maintained in a nonequilibrium state. In the theory of phase transformations under radiation exposure, the appearance of segregation of atoms of a certain kind on the surface of the sample is known as the reverse Kirkendall effect [107] to the generation during exposure in the near-surface layer of a large number of nonequilibrium point defects (vacancies and interstitial atoms) and their subsequent migration along the sample in the direction of effluents. In this case, the separation of the alloy is achieved as a result of the difference in the different grade atoms' diffusion mobility.

According to the model [108], the triple joints of grains have positive or negative dilation, which is modelled by wedge disclosure. With a constant sample volume, positive and negative dilatations are compensated, with areas with positive dilatation acting as sources and the latter as sinks of nonequilibrium vacancies. Thus, the position of vacancies in the space of sources and sinks is not arbitrary but correlates with the quasi-periodic distribution of stress concentrators. Similar ideas formed the basis of models linking the decay of alloys during plastic deformation with the inverse Kirkendall effect [109].

An important conclusion of the work [109] is the possibility of ‘freezing’ the nonequilibrium inhomogeneous state of the alloy achieved with SPD for a long time after the mechanical activation termination. It is possible, if the maximum concentration of nonequilibrium vacancies achieved during the process, is much higher than the equilibrium concentration of vacancies in the absence of mechanical activation. The conclusion is valid under the assumption of an exclusive vacancy diffusion mechanism, which in the theory of diffusion in solids is considered well suited to the reality for substitution alloys.

The researchers’ appeal to the phenomenon of intercrystallite adsorption for the interpretation of phase transformations during plastic deformation of alloys is due to experimental facts indicating a strong distortion of the lattice in the region of grain boundaries and triple joints and the presence of a close connection of the discussed phenomena of phase transformations with grain size. At present, the surface phase transformations are well known and have been studied in detail in isolated samples. At the same time, intercrystallite internal adsorption in nanocrystalline samples obtained by SPD may have specifics related to the features of the achieved structural state [110].

The most promising model of joint segregation of impurities of two grades on surfaces belongs to Guttman [111]; then, it was transformed and discussed by several researchers [112, 113]. An essential feature of this model is the consideration of the interaction of atoms of different grades located in the adsorption layer. Interesting works [114, 115], where segregation from the grain of finite sizes and features of joint surface segregation of impurities of different types to the presence in the adsorption layer of the interaction between impurity atoms of both the same and different varieties are considered. In these works, it is shown that grain size is an essential factor determining the kinetics of segregation and the degree of decay achieved over long periods, and the observed phenomena of competition or cooperation of impurities of different varieties can be accompanied (depending on temperature, the ratio of the initial concentrations of impurities in the volume of the material and the energies of their interaction) by the non-monotonicity of the segregation process, and a strong delay in its up to the formation of intermediate nonequilibrium long-lived phases on the interface surfaces.

In Ref. [116], a model of solid solution decay under large plastic deformations due to the Koehler–Cottrell mechanism was proposed. According to this mechanism, the regions of positive and negative dilation of the crystal lattice are filled with atoms of different grades to the difference in the atomic radii of the alloy components. The authors assign a primary role in the disintegration process of a solid solution to the disclinations of different signs in the area of triple joints of nanoparticles. Earlier in Refs. [117, 118], the kinetics of the formation of impurity atmospheres in the vicinity of edge dislocations was considered. Estimates of the interaction energies between impurity atoms and structural defects [119–125] show that the values of these energies are comparable to the activation energy of diffusion. Not only experimental facts lead to this conclusion, but also the results of the gradient theory of elasticity.

When we analyse the alloys' phase transformations flowing under SPD, especially in the case of torsion under pressure, it is necessary to take into account that the alloy phase diagram depends on pressure; so, it is impossible to use a diagram taken under normal conditions. Neglect of this fact may lead to the erroneous conclusion that the observed phase transformations do not correspond to the equilibrium phase diagram, and is provoked by specific reasons related to plastic deformation.

Many authors, *e.g.*, in Refs. [126, 127], pay attention to the fact that a solid body at SPD is an open-energy system maintained in a non-equilibrium state. If the equilibrium state of the system is determined by the values of the state parameters (at given temperature and pressure) [128, 129], then, the stationary modes achieved during external action should be determined by the intensity of the impact. At the same time, stationary structures become those that provide full dissipation of the energy supplied to the system (in unit time): the so-called dissipative structures [130]. It is essential for their occurrence, the intensity of external influence must exceed an assertive critical value, at which the substance loses the ability to restore permanently its natural phase structure. In addition to the above-mentioned reverse Kirkendall effect associated with the generation of flows of nonequilibrium vacancies at grain boundaries and junctions during SPD, other mechanisms of the alloys' exit from the equilibrium state are possible.

Thus, in Ref. [129], representations were formulated according to which phase transformations with a change in composition in SPD proceed as relaxation from an amorphous state. The passage of partial and zone dislocations is accompanied by permutations of atoms and a violation of the short-range order, up to amorphization. This process is provided by the energy of plastic deformation, as a result of which the system moves away from thermodynamic equilibrium. In regions with the disordered arrangement of atoms, the diffusion mobility is increased, and the chemical potential and, consequently, the solubility of the elements change. These ideas were repeated independently in Ref. [131] and experimentally confirmed in Ref. [132] on an example of the Fe–Cu system. According to the ideas developed in recent works, even in the equilibrium state, the interphase boundary is represented as an amorphous phase layer. The deformation leads to additional amorphization of the boundary regions, in other words, to the broadening of the phase layer, and the relaxation of the deformed state proceeds by the thermodynamics of its decay. Thus, the mechanical fusion of Fe–Cu is presented as a result of the combined action of the processes of deformation and relaxation of interphase boundaries. The possibility of applying the models [129, 131, 132] to explain the decay of alloys at SPD is unclear.

5. Conclusions

A huge and continuously increasing number of works, both experimental and theoretical, have been devoted to studies of the extremely important problem of the evolution of meso- and microstructure (including grain and subgrain structures) [133], as well as phase transformations in the processes of thermomechanical and intensively plastic processing of metals and alloys [134, 135]. This article offers a brief overview of publications containing mainly the results of theoretical research based on models of various levels obtained in the last 20–30 years. The greatest attention is paid to the analysis of changes in the grain (subgrain) structure in the processes of intense plastic deformation; structural rearrangements caused by dislocation-disclosure mechanisms and diffusion (recrystallization) are considered.

The analysis of experimental facts reveals a genetic relationship between phase transformations of different nature. It follows that most of the unusual features of phase transformations (including those in SPD-treated alloys) that do not correspond to the equilibrium phase diagram may be related to disturbances in the lattice structural state in the interface region. Experiments indicate that the peculiarities of the surface states significantly change the thermodynamics of transformations in larger samples, up to 10–20 nm in size; this is most likely due to the long-range nature of the atom interaction. Therefore, the representations developed for phase transformations in nanoclusters can be partially applied to nanograin materials obtained by plastic deformation.

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СТРУКТУРНО-ФАЗОВІ ПЕРЕТВОРЕННЯ В СТОПАХ ЗА ІНТЕНСИВНОЇ ПЛАСТИЧНОЇ ДЕФОРМАЦІЇ

Незважаючи на велику кількість праць, присвячених структурно-фазовим перетворенням у стопах, до сих пір відсутнє повне розуміння картини фазових перетворень за інтенсивної пластичної деформації. Це зумовлено певно тим, що пластична деформація являє собою складний багаторівневий процес, в якому залежно від температури й інтенсивности оброблення діють різні мікроскопічні механізми. Хоча механізми фазових перетворень активно обговорюються в останні десятиліття, та досі залишається актуальною задача класифікації таких перетворень і виявлення основних механізмів реалізації їх залежно від зовнішніх умов.

Ключові слова: стопи, структура, пластична деформація, перетворення.