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NUCLEATION OF RECRYSTALLIZED GRAINS IN METALS DURING THERMOMECHANICAL PROCESSING

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ABSTRACT

In the last 15-20 years, mathematical models have become the most important “tool” for development and creation of technology of thermomechanical processing of metals and alloys due to the occurrence of new class models based on physical theories which replace macrophenomenological models based on macro experiments. Among the founders of crystal plasticity are G. Taylor, G. Bishop, R. Hill, T.G. Lin and others. Many others researchers from the Soviet Union and Russia made a significant contribution to the development of this scientific direction, they are R.Z. Valiev, Ya.D. Vishnyakov, S.D. Volkov, O.A. Kaibyshev, V.A. Likhachev, V.E. Panin, V.V. Rybin, T.D. Shermergor and others. A physically based approach requires a deep understanding of the internal mechanisms and processes that accompany thermomechanical effects caused by inelastic deformation at different scale levels. One of the most important processes for the microstructure formation (and thus for mechanical properties) of finished products obtained by thermomechanical processing methods is the process of recrystallization. In this regard, this article provides an overview of the existing theories of recrystallization, special emphasis is given to nucleation of recrystallized grains. Basic physical mechanisms of nucleation of recrystallized grains are the mechanism based on the classical theory of fluctuations suggested by E.J. Beck and D. Turnbull; the mechanism of nucleation and growth of polycrystal subgrains formed as a result of polygonization (R.W. Cahn, P.A. Beck, A. Cottrell, W. G. Burgers); P.A. Beck’s and P.R. Sperry’s mechanism of grain boundary migration that initially exists in the polycrystal; 4) the mechanism of nucleation and growth of new grains as a result of coalescence of polygonized subgrains (H. Hu, J.C.M. Li, H. Fujita). Implementation of one of these mechanisms of new grains formation depends on the current state of the defective structure resulting from the history of thermomechanical deformation. The analysis of the existing models describing the inelastic deformation under high temperatures shows the need for consideration and inclusion of high-temperature processes, which accompany plastic deformation, in the models describing physical mechanisms.

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1. Introduction

A significant amount of parts and structures produced from metals and alloys and used in aircraft engineering, mechanic engineering, shipbuilding, medicine, and many other areas is subjected to thermomechanical processing (TP) at the last stage of production [1-6 and many others]. When polycrystalline materials are heated, they reveal processes of recovery, polygonization and recrystallization causing changes of a number of physical properties that are usually similar to properties of metals before deformation [7]. Some metals such as most titanium alloys cannot be exposed to deep plastic deformation without heating to high temperatures [2]. Implementation of the mentioned high-temperature processes that can change phase composition of metals (when deformed under an initial temperature above the phase-transition temperature) provides a flexible tool for creating materials with certain required properties [8, 9]. During thermomechanical processing of metals and alloys, meso - and microstructure of the material may evolve significantly. The average grain size, morphology, mutual arrangement, orientation, type of boundaries as well as dislocation substructure change significantly as well [7, 10-13, etc.]. Interaction of heterogeneous phases is an important factor for recrystallization process in multiphase materials [14-16].

It is a well known fact that the state of the internal structure has a decisive impact on mechanical properties of polycrystalline materials [7, 17, 18]. Recrystallization is accompanied by a change of a number of physical properties and structure of the material. First of all, the shape and size of the grains change. The nature of changes depends on temperature, value of deformation, chemical composition of an alloy, initial grain size, etc. [7, 12]; recrystallized fgrains usually have an equiaxial form [19]. During recrystallization, there is a sharp decrease in dislocation density, which causes softening of the material (yield strength decreases). Recrystallization texture occurs, new grains have a preferred orientation caused not only by external load, but also by the conditions of heat treatment, as well as by the previous or current deformation [20]. In this case, orientation of new recrystallized grains is not random, it obeys some relations similar to relations of solid-state phase transitions [20-23]. Consequently, mathematical modeling of thermomechanical processing of metals taking into account recrystallization process is proved to be relevant. During processing, a number of adverse macro effects is noticed, such as folding of the sample, cracks formation, "wrinkling" [6]; mathematical modeling methods can also be used to solve these and other problems.

Currently, there are many mathematical models that describe processes of TP, e.g. single-level macrophenomenological models which are based on experimental data, or first type direct models that explicitly determine grain/subgrain structure, second type models that use a statistical approach to describe macro response [24, 25], or models that use the thermodynamic approach and molecular dynamics. For example, the work [26] provides a mathematical macrophenomenological model to describe visco-plastic behavior of AMg6 alloy under the temperature of 300 °C, taking into account the process of dynamic recrystallization in the deformation rate range of 10-25 s^{-1}. Works [2, 27] report on macrophenomenological models based on the analysis of the experimental data on quasi-static isothermal compression of up to 60 % in wide temperature ranges from 1023 to 1323 K of samples made of Ti–6Al-4V titanium alloy. The classical Johnson–Mehl–Avrami–Kolmogorov model (JMAK) is used to describe the kinetics of recrystallized grains [28-32]. Works [6, 20] report on direct physical models of the first type used to describe inelastic deformation of titanium alloys. Physical models of the first type described in the works [33, 34] and used to describe the behavior of metals with a hexagonal close-packed lattice are similar to the above mentioned models. The difference is the fact that they use probabilistic approach embedded in the cellular automaton for the position of boundaries of new grains (Monte Carlo method). The work [14] reports on a first type direct model based on the physical theory of plasticity used to describe the inelastic deformation of two-phase titanium alloy IMI834 taking into account recrystallization process. The model is encapsulated within the Abaqus software package and subjected to compression tests under isothermal conditions. The work [35] provides information on modeling using method of molecular dynamics of the motion of high-angle boundaries in crystals of niobium, which contain impurity atoms of copper. The authors of this work examine the segregation of foreign copper atoms in grain boundaries and their impact on the diffusion rate of boundaries. The authors believe that this diffusion mechanism is the main mechanism in the recrystallization process of Nb-Cu alloy during annealing. The work [36] provides the analysis of a thermodynamic model which describes dynamic and static recrystallization during deep plastic deformation. The model takes into account a change of the dislocation density in the grain and change of the average grain size, because these parameters are essential for the studied processes. They can be observed and measured during experiments. The work [37] provides a description of a static recrystallization process based on the first type direct model of physical theory of plasticity and phase field theory. In comparison with the most existing models of this class, this solution method is based on the Fourier transformation, and not on the finite element method (FEM). The authors believe that this method is 25-40 times more efficient in terms of computational efforts than the finite element method with a similar degree of accuracy. By summarizing the existing models, it is possible to emphasize their main disadvantage which is the lack of deep and detailed analysis of physical causes of the analyzed high-temperature processes that plastic deformation is accompanied by. The purpose of this work is to describe and analyze mechanisms of formation of new recrystallized grains in metals and alloys with the subsequent possibility of their

application in physically based models of inelastic deformation [38].

2. Main Definitions and Classification of Recrystallization Processes

The term of recrystallization is often found in the works of metal physicists. We would like to quote the most common definitions. The work [11] defines recrystallization as "localized changes in the material that spread from a small number of nuclei due to the movement of the migrating boundary, which absorbs dislocations in the plastically deformed matrix, resulting in formation of more perfect grains than the ones after polygonization". The authors of the work [7] define recrystallization as "occurrence of new grains as a result of heating the deformed material; the occurrence of new equiaxial grains instead of the oriented structure (primary recrystallization)". In the work [12] recrystallization is defined as "the process of nucleation and growth of new grains, in which a stress free nucleus begins to grow in a deformed metal, when the temperature becomes high enough, and gradually absorbs the entire deformed matrix". In the monograph [10] recrystallization is defined as "the process of complete or partial replacement of grains of a specified phase containing certain structural defects by other more perfect grains of the same phase in polycrystalline solids. This process is carried out by formation, or by formation and movement, or only by movement of high-angle boundaries".

The work [7] provides a general description of the recrystallization process. During heating to a certain temperature (recrystallization temperature) for a specified intensity of prior plastic deformation, nuclei of new grains start forming and growing in areas with high deformation of the lattice (boundaries of deformed grains, boundaries of twins, intersections of glide planes, shear strips and other defects). The lattice of new grains is almost not deformed, has a much lower density of defects and is usually separated from the rest of the matrix by high-angle boundaries. The process of grain growth is mostly carried out by diffusion, the atoms of deformed grains attach to the nuclei. In comparison with the recovery process, recrystallization process is more energy efficient, since it is accompanied by a decrease in free energy. In the literature sources used as reference (e.g. see [10]) one can find the classification of recrystallization by the type of applied loads. Prior plastic deformation and subsequent temperature exposure without active deformation loads lead to the so called *static recrystallization*; during hot plastic deformation (simultaneous exposure of external loads and temperature) *dynamic recrystallization* is carried out; after hot deformation and with no deformation load by rapid growth of recrystallization centers prepared during deformation *post-dynamic recrystallization* is carried out. After primary recrystallization is completed *collective recrystallization* can occur during subsequent heating (when some recrystallized grains expand at the cost of other recrystallized grains). The mechanism involved is the migration of high-angle boundaries, when grains with concave boundaries absorb grains with convex boundaries [7]. The reason for such recrystallization is the reduction of grain boundary (surface) energy due to the reduction of the boundary length while grains grow and larger grains occur. The result of heating after primary recrystallization may be different, as parts of grains have favorable crystallographic orientations, which is better for a further growth, others have a lower concentration of defects (the value of volumetric internal energy), a higher mobility of grain boundaries due to inhomogeneous distribution of impurity atoms. Due to the above mentioned processes, many fine-grained crystallites and a small number of coarse-grained crystallites occur, which is called *secondary recrystallization*.

Dynamic recrystallization can involve two different mechanisms: discontinuous dynamic recrystallization (DDRX) and continuous dynamic recrystallization (CDRX). Discontinuous recrystallization is carried out by nucleation of new grains in areas of substantial deformation of lattices (boundaries of phases, grains, and twins, shear strips) and their subsequent growth. This process occurs in materials with low stacking fault energy (SFE), when the process of dynamic recovery is very complicated. Occurrence of a new crystallite and its further growth are caused by the difference of dislocation density in adjacent grains, which is assumed to be proportional to the stored energy [13, 39]. During plastic deformation, the dislocation density increases in new grains, therefore the driving force of the boundary growth decreases and recrystallization stops. Another factor that slows down the growth process is the collision of growing grains during migration of boundaries [13].

Continuous dynamic recrystallization occurs in materials with high stacking fault energy, which allows the recovery process to be completed. This recrystallization can be carried out by many ways [13]. The first of them is called geometric dynamic recrystallization (GDRX) and involves the following processes. During plastic deformation in crystals a dynamic recovery occurs, which causes sub-grain formation; grain boundaries become "jagged" and "wavy", which increases disorientation between the grains. Further intensive plastic deformations gradually "lengthen" grains with high-angle boundaries containing fragments of small-angle boundaries, until their thickness becomes comparable with the fragments. Then the interpenetration of grains occurs, which modifies high-angle boundaries. The result is formation of small equiaxial grains comparable with fragments by size but with high-angle boundaries. Another method of "alternative" recrystallization is carried out due to the active re-orientation of sub-grains with no migration of grain boundaries [13]. In this case successive re-orientation of sub-grains beginning from grain boundaries takes place, which means that sub-grains in the center of the grain can keep the same orientation and have high-angle disorientation at the boundaries. This process is called the

rotation dynamic recrystallization (RDRX). The above-mentioned mechanisms can be implemented simultaneously and are difficult to separate from one another in experimental researches. Another mechanism of continuous recrystallization involves the several processes [40], i.e. under conditions of low strain intensities (about 5-10 %), the cellular structure is formed as a result of self-organization of dislocations during plastic deformation. Vague "thick" cell boundaries are formed with a low dislocation density. As a result of further deformation, boundaries become narrower, dislocation density of the cells decreases, and dislocation density in the boundaries increases, small-angle boundaries of the sub-grains (cells) turn into high-angle ones and their migration rate increases sharply. It is assumed that nuclei of recrystallization centers are the most disoriented, perfect, large cells that grow due to the surrounding sub-grains.

Most of the currently known mechanisms of recrystallization involve nuclei formation of new grains. In order to initiate recrystallization process, it is necessary to fulfill a number of conditions for nucleation of recrystallized grains and their further growth. First of all, recrystallization process depends on the following factors [7, 10-12]:

1. Intensity of cumulative plastic deformation. There is *threshold deformation* for each kind of material during which the process of primary recrystallization becomes possible.

2. Deformation temperature. The recrystallization process is thermally activated and the higher the temperature is, the faster it occurs.

3. Purity of material. Recrystallization of cleaner materials usually occurs at lower temperatures due to the tendency of foreign atoms to segregate at internal boundaries of the crystallites under higher temperatures, which leads to a more difficult migration of boundaries.

4. Initial grain size. Recrystallization process occurs more easily in fine-grained materials, since their boundary area is larger per unit volume, than that of coarse-grained materials. Intercrystalline boundaries are the places of nuclei formation of new grains.

5. Orientation of adjacent crystallites. Mobility of the boundaries depends on their type (simple, special), and on the angle of disorientation (small-angle, high-angle).

3. Physical Mechanisms of Nucleation of Recrystallized Grains

For any mathematical description to be correct, it is necessary to understand the mechanisms of nuclei formation of new grains. Researchers specify up to four of the most known physical mechanisms of new grain nucleation [41]:

1. Mechanism that the classical theory of fluctuation [42] is based on, modified to describe recrystallization processes.

2. Mechanism of nucleation and growth of sub-grains of polycrystal, formed in the result of polygonization process [43-46].

3. Mechanism of strain induced boundary migration (SIBM) suggested in the work [47] and improved in works [48, 49, etc.].

4. Mechanism of nucleation and growth of new grains as a result of coalescence of polygonized sub-grains [50-52].

Let us briefly describe these mechanisms of nucleation and formation of new grains. The classical mechanism of nucleation developed for phase transitions is often used to describe the mechanism of nucleation of new grains during recrystallization process [42, 53]. According to this mechanism, nucleation of new grains occurs due to thermal fluctuations of atoms, which lead to the occurrence of small-sized defect-free crystallites with high-angle boundaries. Such nuclei are stable, if energy difference between the deformed crystal and the nucleus exceeds the surface energy of high-angle boundary. Within this theory, one can take into account the incubation period of formation and define the position of nuclei in the material, as areas with high gradients of movements, which are the most likely places for nucleation of new grains. It is noted that places, which permit nucleation, exist before recrystallization process and are not nuclei themselves in the strict thermodynamic sense.

Probably, one of the first researchers who attempted to describe the mechanism of new grains formation was W.G. Burgers (see the work [44]), then his idea was developed in the work [54]. W.G. Burgers analyzed experimental data on geometric shape of recrystallized grains [55] and suggested the mechanism of nucleation and further growth of recrystallized grains (term "nuclear spot" is used in the article), which explained two experimental facts: 1) different nuclei observed in a polycrystal have different formation periods (incubation periods); 2) different nuclei grow with different rates. Another significant requirement for the developed physical model is the description of the simplified geometry of recrystallized grains at a first approximation.

By using the experimental data on accumulated elastic energy [23], W.G. Burgers assumed that the polycrystal is divided into zones, that have more deformed areas with high stored energy and less deformed areas with low energy. Areas with low energy are called blocks with the size from 0.1 μm. Between blocks there are thin narrow layers with high elastic energy that are called "transition layers" in the quoted work. A combination of blocks with transition layers is called mosaic blocks. Blocks are disoriented relative to each other in this structure. Atomic structure in transition layers differs from the structure of blocks or that of original grains. According to the author, the question of structure of such bands is extremely important, but not studied enough at that time. A block with less stored energy and good orientation relative to adjacent blocks can begin to grow deep into other blocks, i.e. this block is the nucleus of a new grain. Nuclei grow by moving the transition band by means of diffusion mechanism. In other words, the transition area is "pushed" deep into adjacent blocks.

Fig. 1 schematically shows the process. It is assumed that grain *A* subjected to recrystallization with a nucleus at point *a* grows in all directions with the same rate. Places of new nuclei formation correspond to areas with low energy. At some point, cross section of the new crystal will be a circle of radius *r*. Dimensions and shapes of new growing crystallites are determined in the first place by the distance between adjacent nuclei and by their growth rate.

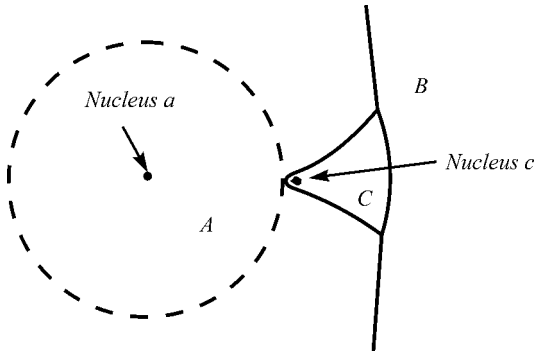

Fig. 1. Schematic representation of nuclei formation and growth [54]; *a*, *c*: nuclei of new grains; *A*, *C*: grains subjected to recrystallization; *B*: original grain of polycrystal

According to experimental data on grain structure of recrystallized grains, a hypothesis is developed that some of the nuclei of new grains (nucleus *c* in Fig. 1) do not begin to grow until the point when the new crystallite *A* comes close to the nucleus *c*. Crystallite *A* is called the stimulating crystallite. Thus, growth of one grain provides an increase of the gradient of stored energy and can initiate growth of the nucleus in point *c*. It is noted that polycrystal has a certain recrystallization texture after recrystallization, therefore nuclei must have a specific orientation that is good for further growth. This work does not provide a detailed discussion of these orientations.

One of the disadvantages of the suggested mechanism [54] of nucleation of recrystallized grains is the lack of detailed analysis of physical mechanism for describing the occurrence of a "block" structure with different stored energy and defects concentration. This problem is analyzed in the work [43], which notes that the most reasonable mechanism of new grains formation is given in the article [56]. According to the suggested mechanism, a crystal's areas, which are most probable for nucleation of recrystallized grains, are the areas with high local stresses caused by a high concentration of crystal lattice defects. The disadvantage of this theory [56] is the assumption, that for nucleation, it is necessary that a small area with high stresses spontaneously turns into an area with low stresses. In this case, an experimental fact that number of nuclei increases as deformation increases can be easily explained. The theory of nucleation in areas with low stresses suggested by W.G. Burgers [54] does not describe this fact. The mechanism [56] has one significant disadvantage, as there is no physical explanation for local stress relieving. The authors of the work [43] suggest to correct this disadvantage by using the phenomenon of polygonization, discovered by that time [57]. As a result of the polygonization process during plastic deformation, elastic energy stored in the polycrystal allows for stress-free areas to occur, which are separated by sub-boundaries with an increased dislocation density. Stress-free areas of crystals attach to areas with high stresses where polygonization process did not occur. Defect-free areas (fragments) start growing deep into more defective ones. It is being noted that for further migration of the boundary, nuclei must be specifically oriented relative to the rest of the environment. It is suggested that the number of good oriented nuclei of new grains is not large, therefore not all of the nuclei of crystallite immediately start growing deep into adjacent grains. This corresponds to the experimental data on incubation period and a further increase of the nuclei number with an increase of annealing time by the exponential dependence [58].

Many researchers that work in this field believe that one of the most physically based mechanisms of recrystallization is described in the article [45]. It is the author's opinion that the main reason for recrystallization is the presence and movement of dislocations during pre-plastic deformation. It is believed that nuclei of recrystallization grains are formed during inelastic deformation and occur in areas of lattice deformation with local inhomogeneities, for example, in shear strips, twin layers, and grain boundaries. The author believes that recrystallization is always preceded by polygonization, which results in formation of many disordered sub-areas or fragments (polygons). The fragments are disordered to a small angle relative to the parent grain but are almost free from defects. It was experimentally found that during subsequent annealing some of the fragments can absorb adjacent ones. The probability of fragment growth is higher, the bigger the local curvature of the lattice (formed as a result of polygonization) is. Using the suggested mechanism, kinetics of the growth of new grains is described; the modelling results are close to those obtained using Johnson-Mehl-Avrami-Kolmogorov models.

It is noted in the work [59] that the Cahn mechanism [45] is not completely correct for several reasons. According to the mentioned mechanism, the migration of boundaries begins in the areas adjacent to small-angle boundaries, and during recrystallization, the migration rate of the boundaries decreases, but the angle of disorientation of fragments, on the contrary, increases. It does not correspond to the experimentally known fact that a high rate of boundary migration is noticed in the areas adjacent to high-angle boundaries. The results of the experimental researches [60] show that sub-grains/fragments are not nuclei of new grains. According to the mechanism suggested in the work [45], recrystallization can occur in monocrystals. However, experiments on plastic deformation to the value of about 100 % and subsequent annealing under homologous temperature of about 0.5 using polycrystalline and monocrystalline samples of aluminium [61] and copper

[62] show that in comparison with polycrystals, monocrystals are not recrystallized.

Therefore, the authors of the work [59] suggest their own mechanism of recrystallization, the primary role in which is played by grain boundaries. This mechanism is based on formation of "ledges" at grain boundaries due to an incompatibility of slip systems of shears. In the area of the ledge a nucleus is formed, oriented to several degrees with respect to the original grain (see Fig. 2). Similar to works [63, 64], it is assumed that new grain growth is driven by the difference in stored energy on both sides of the high-angle grain boundary. It should be mentioned that in comparison with the mechanism [45], the presence of fragments is not supposed for recrystallization, and the authors of the work [63] do not suppose the presence of nuclei.

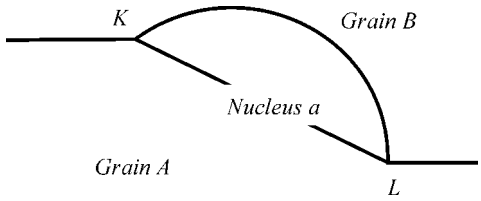

Fig. 2. Schematic representation of formation of nucleus *a* by bending the ledge *KL* from grain *A* to grain *B* with higher stored energy [59]

The work [65] motivated many researchers to perform detailed studies of both static and dynamic recrystallization. The mentioned work provides the description of annealing of technically pure aluminum polycrystal, which was pre-deformed by rolling by 40 %. As a result, new grains growth was observed. In addition, the authors found a prevailing direction of growth of nuclei turned by an angle of 40° relative to crystallographic direction <111> of the original matrix. This allowed to develop a hypothesis, that, as a result of recrystallization, only those nuclei occur that are oriented for further growth [65]. In the foreign literature this theory is called the oriented nucleation theory. According to another hypothesis, which was developed much later [47, 66], good oriented grains have the most rapid growth rate among differently oriented nuclei (oriented growth theory). These grains are the ones that grow deep into adjacent grains.

The article [66] discusses the problem of the primary contribution to the development of texture of recrystallization of oriented nucleation and growth of new grains. The following experiment was conducted for this purpose. Two scratches were applied to the surface of the aluminum polycrystalline pre-annealed for 4 hours at a temperature of 650°C and pre-deformed by rolling by 12 %. After that annealing was carried out for one hour at a temperature of 350°C. As a result, differently oriented statically recrystallized grains were found in areas of increased local deformations where scratches were applied (see Fig. 3).

Results of the experiments given in the work [66] allow us to draw the several conclusions, such as 1) the growth rate of recrystallized grains varies over a wide range and strongly depends on the orientation of nuclei; 2) there are specific orientations of the preliminary growth of recrystallized grains in polycrystalline materials (for example, direction <111> rotated by 40-45° relative to the initial orientation in pure aluminum); 3) recrystallization texture is determined by the oriented growth in a greater degree, than by the oriented nucleation; 4) grain growth is an essentially anisotropic process and diffusion is the process that helps boundaries migrate.

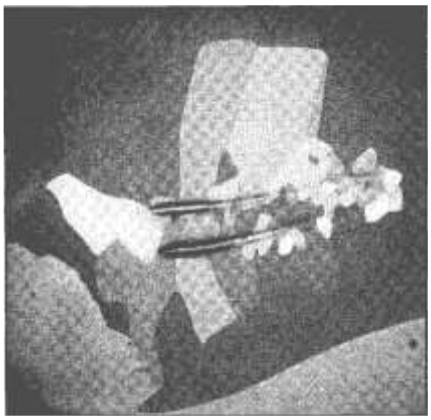

Fig. 3. Differently oriented recrystallized grains after applying two scratches to the surface of technically pure polycrystalline aluminum, subjected to rolling and subsequent annealing [66]

It should be noted that works of Beck and his co-authors [47, 66] allowed to determine an unknown mechanism of recrystallization. In the work [47] it was shown that less nuclei of recrystallized grains occur during annealing of pre-rolled aluminum, as the degree of deformation increases, and at the degree of deformation of 40-50 % there are almost no nuclei. Instead, the formation of volumes free from internal stresses is conducted by a different mechanism i.e. due to strain induced boundary migration (SIBM). Based on this result, the authors of the mentioned work distinguish two different types of grain growth. The first of them (previously mentioned in the work [65]) is the formation of new grains inside the initial grains and subsequent growth in direction to the center of grains curvature approximating the grain boundary (grains *C*, *D*, *E* in Fig. 4, *a*). The second type was not studied previously; it involves "bending" of original boundaries of the polycrystal from the center of grains curvature (SIBM mechanism). An important difference of SIBM mechanism is that nucleation is not required for its implementation. This is confirmed by the experimental data proving an immediate beginning of growth of defect-free areas adjacent to the boundaries of original grains. The usual mechanism of recrystallization takes place after some delay (incubation period) necessary for nucleation of new grains. Another difference of SIBM mechanism is the increase of length of grain boundaries and formation of a special "wavy" ("finger-shaped") structure of grain boundaries (grain *A* in Fig. 4, *b*). Growth of new grains during usual recrystallization (the first mechanism) is

driven by the excess of free energy associated with grain boundaries. In that way grains tend to reduce their free energy, allowing structure to achieve balance and reducing curvature and length of grain boundaries. This is due to absorption of grains with increased energy. The authors of the work [47] believe that boundary movement during strain induced boundary migration is caused by the same reason. This assumption is caused by the fact that an almost defect-free area remains outside the boundary during such boundary movement. The increase of the boundary area is not explained.

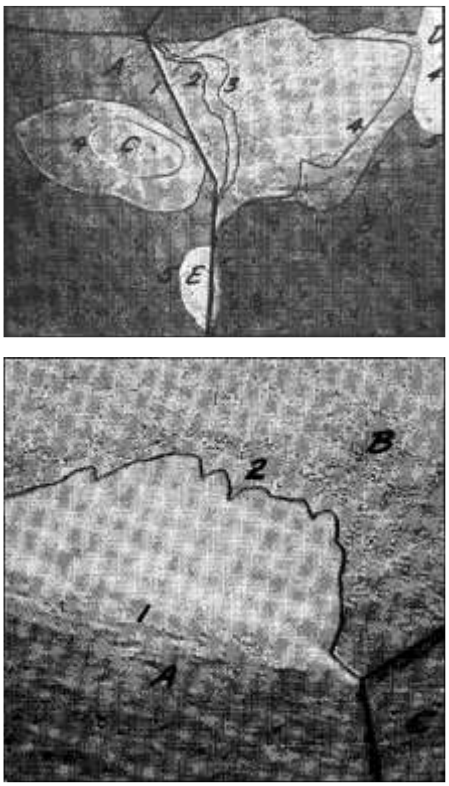

Fig. 4. Boundary growth of grains C, D, E from the center of grains curvature; growth of grain *A* into grain *B* according to SIBM mechanism [47]

The described SIBM mechanism is directly related to the mechanism of nuclei formation of new grains, although it is not reflected in the works of Beck [47, 66]. This relation was described later in work [49]. This is partly associated with the development of equipment that allows to analyze and determine the orientation of crystallites of smaller sizes. The authors of this work identified deformation bands, which had not been possible previously [47, 65]. Three methods of nucleation of recrystallized grains were identified, i.e. 1) in initial boundaries of polycrystal; 2) in "internal" boundaries formed by deformation bands; 3) in areas that can not be clearly identified by researchers but are supposed to be boundaries of deformation bands.

The authors of the work [49] believe that according to SIBM mechanism not only growth of grains is possible, as indicated in the work [47], but also nuclei can be formed. As a result of difference in defects concentration of adjacent crystallites, "ledges" [59] are formed during deformation, which further separate from the original grain and become nuclei of recrystallization (see Fig. 5). The authors of this work point out that such a mechanism of nucleation prevails at deformation degree of up to 20 %, then its importance gradually decreases. At a higher deformation degree, nucleation takes place in deformation bands; according to the authors, the mechanism of nucleation in these bands is similar to SIBM mechanism, but it is not described in detail.

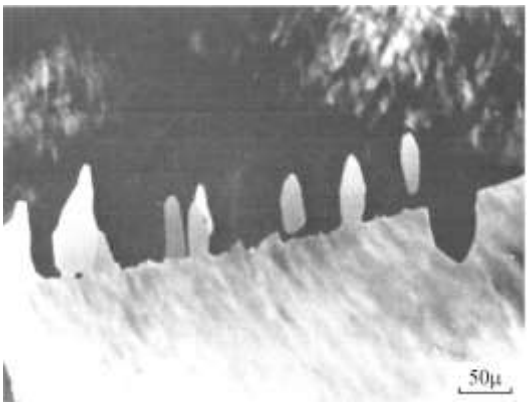

Fig. 5. Nuclei formation of new grains according to SIBM mechanism in aluminium polycrystal which had been deformed by 40 % and annealed during 1 hour [49]

The quoted work describes SIBM mechanism which contains several stages (see Fig. 6), 1) as a result of plastic deformation, energy accumulates on the defective structure in crystals; 2) due to the energy difference, the boundary starts "bulging" towards the grain with more stored energy, a small area outside the growing boundary is almost defect-free; 3) a further growth of a new defect-free grain due to boundary migration; 4) completion of the process and occurrence of a new defect-free grain, the orientation of which is close to the orientation of the old grain, where that growth began from.

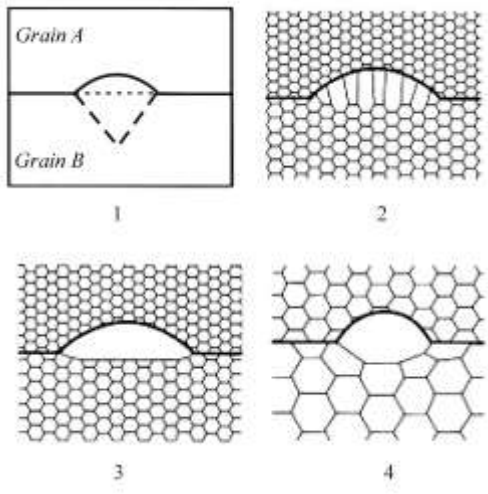

Fig. 6. Schematic representation of nuclei formation according to SIBM mechanism [49]

The above-mentioned mechanism of new grains formation and growth due to bulging of boundaries of initial grains (SIBM mechanism) is confirmed by plenty of experimental data. This mechanism can be implemented in materials with high and medium stacking fault energy. The work [63] describes the experimental studies of plastic deformation of a technically pure silver polycrystal. Thin plate samples (foil) were subjected to cold deformation either by uniaxial tension up to the value of 25 % or by rolling up to the value of 95 %. After that an isothermal annealing in a calorimetric chamber was carried out and energy accumulated during previous plastic deformation was measured. In addition, the state of the dislocation structure was examined using an electronic microscope. It should be noted that two types of experiments are described in the work, when the sample was first annealed, then subjected to electropolishing, after that its surface was studied using the microscope; when the sample was pre-polished; the changes of the dislocation structure occurred immediately at a high-temperature stage (during annealing). At low deformation degrees (of about 25 %) the dislocation structure has a cellular form. The cells are oriented relative to each other at an angle of about 1°. As deformation increases, the angle of disorientation increases as well, and some cells become sub-grains. Dislocation density within the cell boundaries is much higher (about 5 times), than that inside the cells. At high deformation degrees (95 %) polygonization is observed, which was not observed during the deformation of lower degrees. The resulting experimental data testify to the implementation of SIBM mechanism. Firstly, the orientation of the new grains is close to the orientation of the original grains. Secondly, only during hot deformation "swelling" or "bulging" of grain boundaries was observed, during cold deformation grain boundaries remained straight. The area outside the bent boundary is almost defect-free with a low dislocation density.

The kinetics of SIBM mechanism was first suggested in the work of Bailey and Hirsch [64]. One of their tasks was to find criteria of growth of recrystallized grains according to SIBM mechanism. The authors of the work suggested that the boundary migration is caused by the difference of free energies f of crystallites adjacent to the boundary. In other words, a part of the crystallite with high free energy is absorbed by another part with a lower level of free energy, i.e. only due to this process, the total free energy of two crystallites should be reduced. It is also necessary to consider the changing of intergranular energy of the boundary:

$$f\Delta v = e\Delta v - \gamma\Delta s, \quad (1)$$

Δs is the increase of the boundary area during changing of grain volume by the value of v, e is difference of energy accumulated in the grains, γ is energy of intergranular boundary. A boundary starts migrating, when the $f > 0$ condition is fulfilled, which means that

$$e > \gamma\Delta s/\Delta v. \quad (2)$$

The authors of the work [67] suggest an original recrystallization mechanism, which according to its description, is close to SIBM recrystallization mechanism. This work contains results of experiments on compression of aluminum samples (Al-5% Mg) at temperatures of 293-773 K in the range of strain rates of 10^{-5}-10^{-1} s^{-1}. During studies of deformed samples using the microscope a structure called "core and mantle" near the grain boundaries was found. A lot of small defect-free grains occur in this structure (see. Fig. 7).

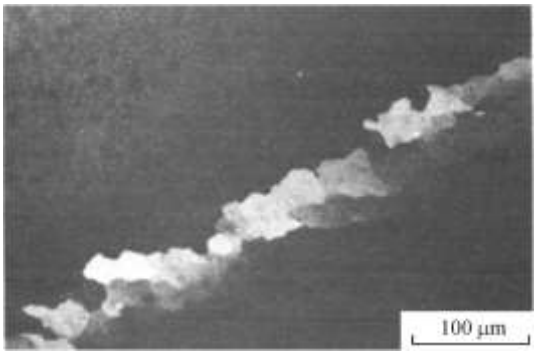

Fig. 7. “Core and mantle” structure in the boundary resulted from aluminium polycrystal deformation (Al-5%Mg), the strain is 0.6, the temperature is 723 K, the strain rate is $2\cdot10^{-3}$ s^{-1} [67]

The authors suggested the mechanism of formation of this structure. It is assumed that the grain boundary sliding is carried out under low temperatures in well oriented boundaries (see Fig. 8). As a result, local stresses near grain boundaries decrease, and stresses near triple junctions (or boundary fractures) (where sliding is difficult) increase. The mentioned work proves the formation of high-angle boundaries, which originate from the triple junctions. Then "irregularities" ("peculiarities") of grain boundaries develop ("bend") due to local boundary migration caused by the difference of dislocation density between the boundaries of adjacent grains. Small irregularities can completely disappear as a result of grain boundary sliding. Otherwise, sliding between the grains can only occur on small areas of the boundary. Continuing plastic deformation will lead to re-orientation of these ledges and subsequent formation of high-angle boundaries. If disorientation is higher than 10°, it is possible to speak about the formation of new recrystallized grains.

In the above mentioned works, SIBM mechanism was studied in the processes of static recrystallization, but it can occur in dynamic recrystallization as well. The work [68] is devoted to the impact of dynamic recrystallization on formation of the polycrystal texture of technically pure copper. The authors of this work conducted experiments on uniaxial compression of samples from the specified material at a temperature of 200-600 °C and a deformation value of 0.1-0.7. It is noted that dynamic recrystallization occurs by bending the initial high-angle boundaries of polycrystal grains according to SIBM mechanism. This mechanism is especially important at the initial stage of recrystallization

and at low degrees of deformation. During the continuing plastic deformation the deformation bands occur in the defective structure. In these deformation bands, the formation of new grains is also possible. Formation of new grains in the deformation bands is more energy-efficient in this situation. During high degree deformations, re-crystallization according to SIBM mechanism is almost not carried out. New boundaries (caused by plastic deformation) "bulge". It is noted that evolution of the texture during dynamic recrystallization is not completely clear.

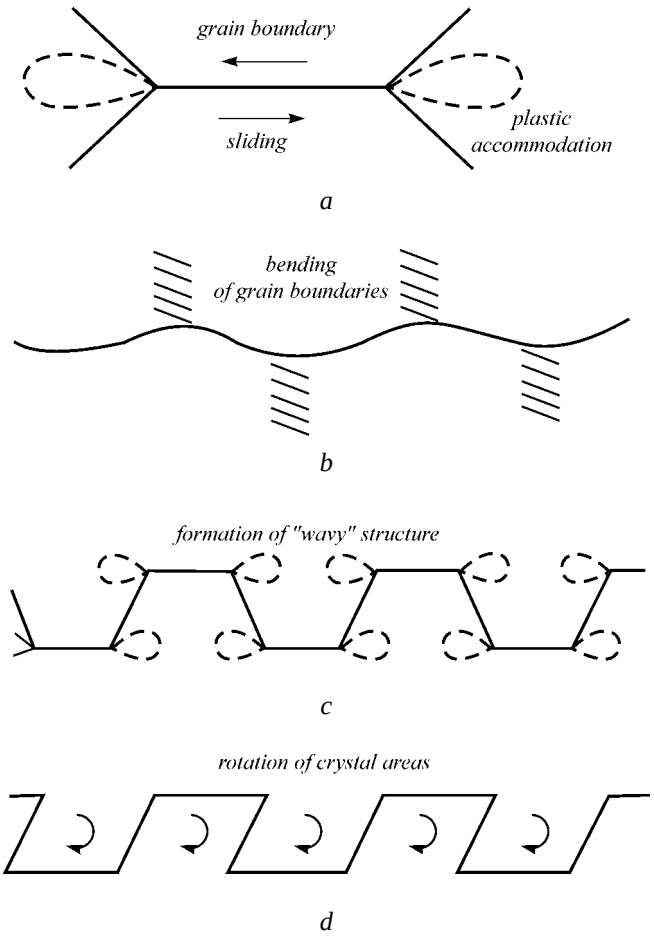

Fig. 8. Schematic representation of formation of recrystallized grains [67]; *a*) process of grain boundary sliding, leading to increased stresses near triple junctions; *b*) bending of grain boundaries caused by boundary migration; *c*) grain boundary sliding in some areas of the boundary and dislocation sliding, leading to "wavy" structure formation; *d*) dislocation sliding in elongated areas, leading to rotation of small areas

The work [69] is devoted to high-temperature uniaxial compression of A286 steel samples (Fe–28Ni–13Cr) at temperatures of 950-1100 °C and low loading rates in the range from 10^{-3} to 1 s^{-1}. It is noted that the recrystallization mechanisms in are greatly dependant on one of the important characteristics of the material, which is the stacking fault energy. This alloy is characterized by a high amount of nickel with a high stacking fault energy, and austenitic phase of steel has a low stacking fault energy. As a result, A286 alloy shows an abnormal nature of σ–ε diagram. The reason for this is the restructuring of the defective structure, where recrystallization plays an important role. The authors of this work emphasize the dependence of the dynamic recrystallization mechanisms on the external loading rate. At low strain rates (10^{-3}-10^{-2} s^{-1}) recrystallization takes place due to the continuous dynamic recrystallization, which is followed by an active dynamic recovery. In this case, the deformation curve (see Fig. 9) does not have a clear peak.

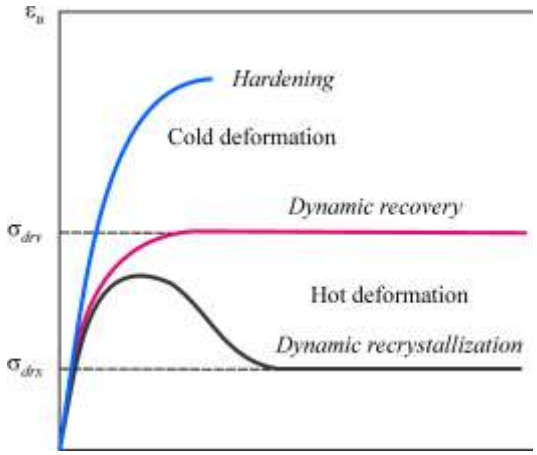

Fig. 9. Typical "σ–ε" is the loading diagram for metals under different temperatures and processes of a high-temperature deformation; σ_{drv} are characteristic stresses of dynamic recovery, σ_{drx} are characteristic stresses of dynamic recrystallization

At higher loading rates, recrystallization is carried out according to SIBM mechanism. In this case, stress drop is clearly seen on the deformation curve, which is associated (in the opinion of the authors) with the formation of a fine-grained "necklace" grain structure at the boundary according to SIBM mechanism and subsequent dynamic recovery in the initial grains. The authors do not specify physical reasons for changing the recrystallization mechanisms at different loading rates.

The work [70] describes plastic deformation and dynamic recrystallization processes in magnesium alloy ZK60 (material with low SFE) (Mg–5.8Zn–0.65Zr) in experiments on uniaxial deformation at temperatures of 423-723 K and loading rates of 10^{-5}-10^{-1} s^{-1}. The authors emphasize the dependence of the recrystallization mechanisms on deformation temperature and plastic deformation mechanisms. They distinguish three types of recrystallization for this type of alloy, such as the low-temperature dynamic recrystallization, which is associated with twinning, basic and a+c (pyramidal) sliding and carried out at a temperature of 473 K; the continuous dynamic recrystallization with an intensive cross sliding, implemented in the temperature range of 473-523 K; the discontinuous recrystallization, which is carried out according to SIBM mechanism simultaneously with dislocations climb at a temperature of 573-723 K. In the latter case, it is experimentally shown that the nucleation of new grains occurs by the migration of boundaries of old

grains with an extensive formation of slip bands. The localization of plastic deformation at a microlevel leads to the formation of ledges at boundaries of the original grains. Moving lattice dislocations are absorbed by low-angle boundaries of the ledges, then turning them into high-angle boundaries. This process is controlled by self-diffusion, which is confirmed by the fact that, as temperature decreases, the size of grains recrystallized according to this mechanism decreases sharply. The authors of the mentioned work emphasize that the plastic deformation and recrystallization mechanisms have a clear relation. SIBM mechanism plays an important role in small deformations, and then formation of grains in slip bands starts.

The work [52] describes coalescence of sub-grains/fragments and its impact on recrystallization. It is noted that during cold plastic deformation of technically pure aluminium polycrystal sub-grains with the size of 0.1 μm occur. Subsequent heating leads to coarsening of the sub-grains by combining them (coalescence). As a result, the size of sub-grains in a stable grain structure is 3-10 μm. The coalescence process is important for recrystallization due to the fact that boundaries of sub-grains are a sink for lattice defects. Since the activation of recrystallization requires a specified value of difference of free energy between nucleus and the main matrix, the latter requires the formation of a stable sub-grain structure. It was experimentally found that 1) sizes of sub-grains begin to increase until the beginning of recrystallization; 2) after recrystallization began, the coalescence of grains slowed down; 3) at the beginning of recrystallization, the boundaries were indistinct and vague. The work [50] describes the rotation of sub-grains during recrystallization and coalescence of sub-grains. It is noted that the rotation of sub-grains, that leads to changing the low-angle boundaries, is more energy-efficient. This process can cause coalescence of sub-grains.

4. Conclusion

This work provides the description and analysis of the nucleation mechanisms of recrystallized grains in polycrystalline materials. The classification of recrystallization mechanisms is given. The implementation of one of these mechanisms of nucleation of recrystallized grains and of their subsequent growth is closely connected not only with applied loads, deformation temperature and their rates, but also with physical properties of the material (stacking fault energy, melting point, phase transition point, elastic interactions of atoms, diffusion of foreign atoms and self-diffusion, crystallography of crystallites, accumulated energy during plastic deformation, thermal conductivity). The prevailing recrystallization mechanism depends on the current state of the defective structure of the material. First of all, this is about the state of grain structure (shape and size of grains, grain boundaries, their morphology, structure, mutual arrangement, length, orientation of adjacent grains), and sub-grain structure (shape and size of fragments, low-angle boundaries of sub-grains). Dislocation/sub-dislocation structure plays an important role for nucleation of recrystallized grains, for it determines the formation of sub-grains and cells, the direction of growth of new recrystallized grains, the formation of defects at the grain boundaries. A good example for the impact of various properties of crystallites and defective structure are recrystallization processes in multiphase materials. For example, in two-phase titanium alloys, recrystallization of α- and β-grains occurs according to different mechanisms. Based on the above facts, it is critical to know, understand and describe the restructuring processses of the defective structure (at higher temperatures as well) in order to build physically based models of inelastic deformation.

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