Rev. Adv. Mater. Tech. vol. 3 no 1 (2021) 29-41
DOI:10.17586/2687-0568-2021-3-1-29-41

Grain Boundary Transformations in Deformed Nanocrystalline Materials: A Brief Review

S.V. Bobylev

[1]Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg 199178, Russia
[2]Peter the Great St. Petersburg Polytechnic University, St. Petersburg 195251, Russia

Received: February 02, 2021

Abstract. The theoretical models describing various grain boundary transformations acting in plastically deformed nanocrystalline materials are briefly reviewed. We demonstrate the important role of grain boundaries and their transformations in the process of plastic deformation of nanocrystalline materials. Theoretical results are discussed and compared with available data of experimental studies and computer simulations.

1. INTRODUCTION

Grain boundaries (GBs) are integral structural components of polycrystals and directly define their physical and mechanical properties [1]. For certain classes of materials, the role of GBs becomes extremely high for one reason or another. Compared to conventional polycrystals (with grain sizes of the order of micrometers) in nanomaterials (NCMs) a much larger fraction of the nanocrystalline (NC) volume is occupied by GBs. Therefore, it is natural to believe that GBs play a significant role in the process of plastic deformation of NCMs. Indeed, majority of mechanisms of plastic deformation in NCMs are controlled by GBs. In particular, GB sliding, Coble creep, and rotational deformation are examples of plastic deformation mechanisms mediated by GBs typical in NCMs [1–3]. The standard dislocation plasticity, which is realized via intragrain slip of lattice dislocations, also undergoes significant changes under the conditions of a nanocrystalline structure. For example, GBs can play a role, which is unusual for coarse-grained polycrystals, as effective alternative sources of mobile lattice dislocations. Under these conditions, the study of the structure of GBs and their transformations is extremely important for understanding the processes occurring in NCMs subjected to the plastic deformation.

This paper briefly reviews various theoretical models developed by author and his colleagues in the Laboratory of Mechanics of Nanomaterials and Theory of Defects at the Institute for Problems in Mechanical Engineering of Russian Academy of Sciences (IPME RAS) over past two decades in the field of GB transformations realized in plastically deformed nanocrystalline materials.

2. GRAIN BOUNDARY TRANSFORMATIONS AND THEIR ROLE DURING PLASTIC DEFORMATION PROCESS

In the process of plastic deformation GBs can play different roles undergoing various transformations and affecting deformation process in different ways. We can divide GBs by their roles in plastically deformed nanomaterials roughly in the following categories:

Corresponding author: S.V. Bobylev, e-mail: bobylev.s@gmail.com

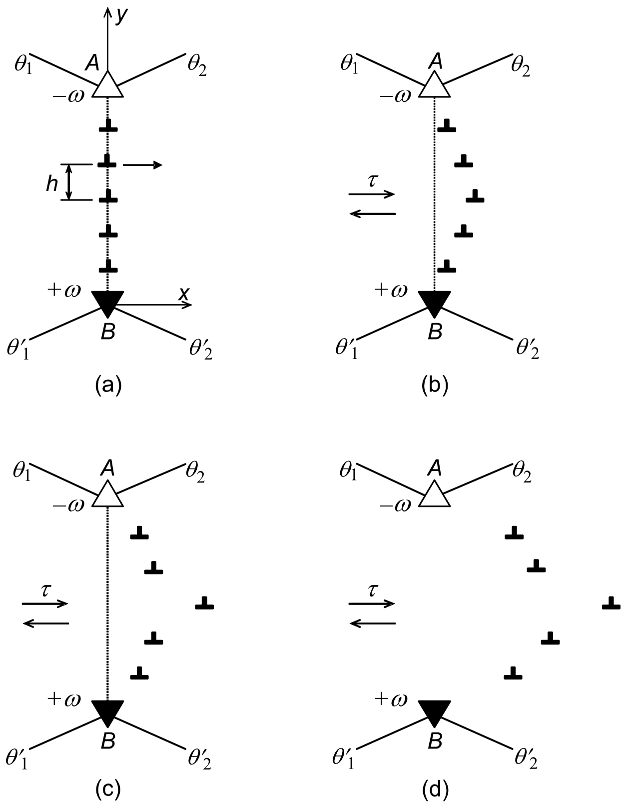

Fig. 1. Decay of a low-angle tilt boundary represented as a periodic dislocation wall terminated at triple junctions A and B. (a) Dislocation wall in its initial state (in the absence of mechanical load). (b) Shear stress t causes bowing of the dislocation wall. (c) One of the dislocations releases from the dislocation wall. (d) Dislocation wall completely decays resulting in formation of a dipole of uncompensated disclinations. Reproduced from [6] with permission. Copyright (2004), Elsevier.

(1) alternative sources of lattice dislocations;
(2) medium for carriers of plastic deformation (usually, GB dislocations);
(3) carriers of plastic deformation themselves as a result of various GB migration processes.

GBs belonging to the first category serve as effective sources of lattice dislocations usually through low-angle GB destruction [4–6] or heterogeneous (originating on GB dislocations) dislocation nucleation processes [6–11]. This type of mechanisms are reviewed in section 3. GBs that can act as medium for plastic deformation (category 2) enable processes like GB sliding and GB diffusion. GB sliding is of particular interest due to being responsible for superplastic behavior of certain NCMs (even at room temperatures), which is highly desirable property for practical applications. These behavior is unusual because GB sliding is plastic shears localized within GBs which normally creates defects – sources of internal stresses – in GB triple junctions capable of initiating the nucleation of nanocracks and subsequent brittle fracture of the nanomaterial [2, 12]. Because of that, GB sliding is usually considered alongside various accommodation processes which are reviewed in section 4. Finally, when it comes to GB migration processes we are interested not only in plastic deformation itself but also in grain growth and grain refinement processes which is often related to the athermal stress-driven migration [13]. GB migration models are described in section 5. Below we consider specific mechanisms, where GBs can perform roles listed above.

3. GRAIN BOUNDARIES IN NANOCRYSTALLINE MATERIALS AS ALTERNATIVE SOURCES OF MOBILE LATTICE DISLOCATIONS

Due to small grain size of NCMs the standard mechanism of plastic deformation – lattice dislocation slip in grain interiors – can be significantly hampered due to suppression of the conventional dislocation sources (Frank-Read sources and the double cross-slip). However, this mechanism can still work quite efficiently if there are alternative sources of mobile dislocations. Many authors reported on experimental evidence of lattice dislocations, both perfect [14,15] and partial [16–18], in NCMs. In the special case of shock-loaded

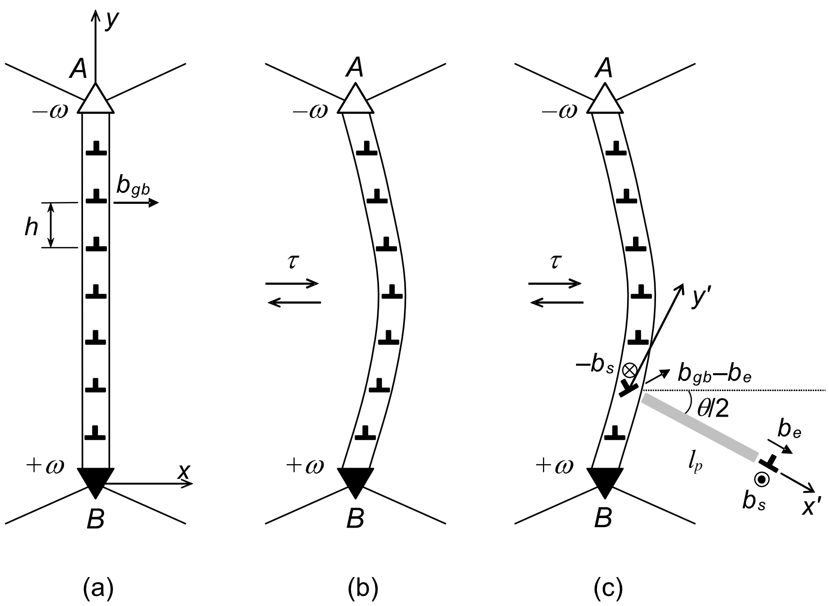

Fig. 2. Evolution of high-angle boundary with dislocations. (a) Initial state. (b) Bowing of boundary under the shear stress action. (c) Shear-stress-induced splitting of a grain boundary dislocation results in both the formation of an immobile GBD and emission of a partial Shockley dislocation into the grain interior. Reproduced from [6] with permission. Copyright (2004), Elsevier.

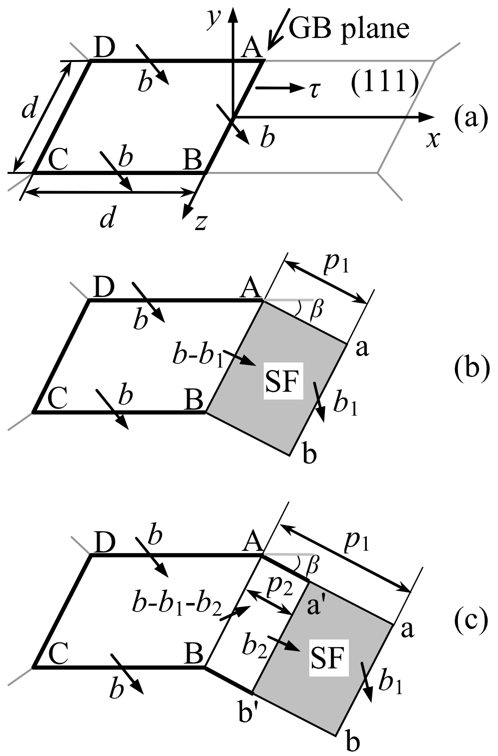

Fig. 3. A schematic illustration of the generation of the dislocation loops with Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ at the preexistent GB dislocation loop ABCD with Burgers vector $\boldsymbol{b}$. Reproduced from [8] with permission. Copyright (2006), The American Physical Society.

nanocrystalline Ni, the density of observed dislocations was extremely high, ~10^{16} m^{-2} [19]. Molecular-dynamics computer simulations demonstrated the generation of partial and extended perfect dislocations by GBs and their triple junctions [20, 21]. These experimental data suggest that GBs are the major alternative sources of mobile dislocations.

A number of different theoretical models were suggested by author and his colleagues to describe heterogeneous nucleation of mobile lattice dislocations on GBs. For example, the decay of low-angle tilt GBs into lattice edge dislocations [4–6], the emission of partial and perfect dislocations by GB dislocations [6–11], GB disclinations [22–26], GB triple junctions [7–9, 27–29].

In particular, Bobylev et al. [4–6] showed that the decay of low-angle GBs (schematically shown in Fig. 1) into ensemble of mobile lattice dislocations in mechanically loaded NC metals causes local plastic deformation in the grain where the decay takes place, as well as in neighboring grains. The decay of one low-angle GB can initiate a chain decay of neighboring GBs and the generation of a shear band (a narrow region where plastic deformation is localized). The critical stress τ_c of GB decomposition characterizes the initial stage of plastic deformation occurring via the development of shear bands. For nanocrystalline Fe, using 2D discrete dislocation dynamics approach, the value of τ_c was estimated to vary from 0.5 GPa (for GB misorientation angle $\omega \sim 2°$) to 2.5 GPa (for $\omega \sim 10°$). Its average value $<\tau_c>$~1.5 GPa coincides with the experimentally measured value of the shear stress [30] at which shear bands are formed in nanocrystalline Fe.

Bobylev et al. [6] also proposed dislocation-based model describing emission of partial lattice dislocations from high-angle GBs nucleated on GB dislocations

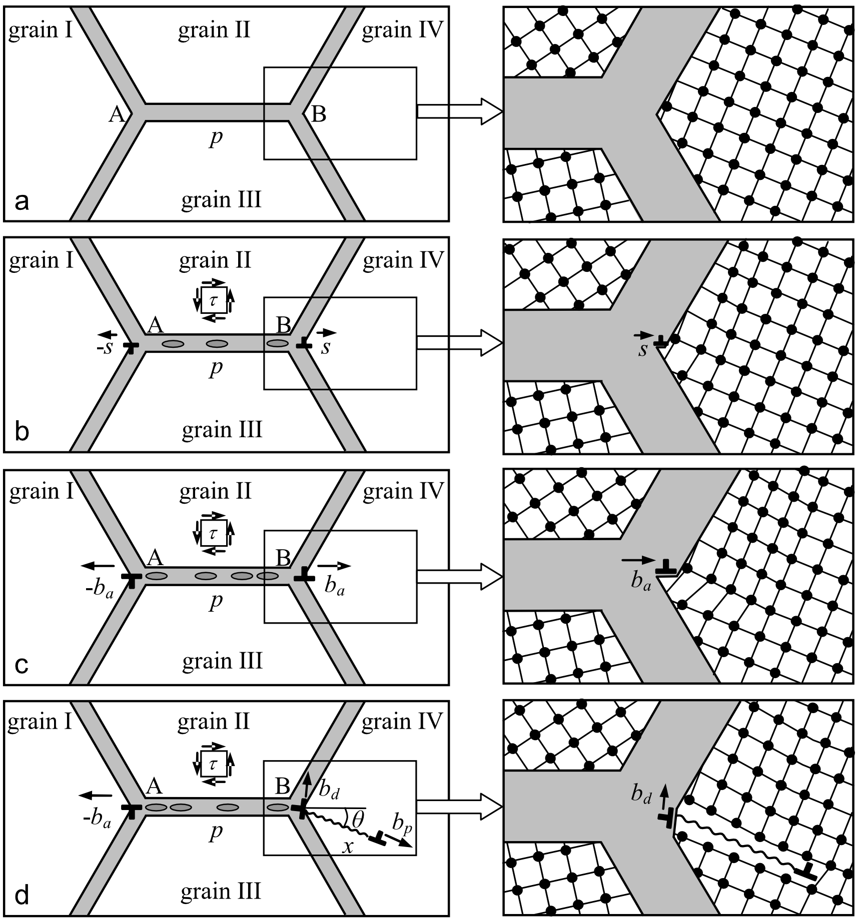

Fig. 4. Generation of dislocation dipole at an amorphous intergranular boundary followed by emission of a partial dislocation into an adjacent crystalline grain in a deformed NC ceramic specimen (schematically). (a) Initial, dislocation-free state. Four grains I, II, III and IV are divided by amorphous intergranular boundaries (grey strips). (b) Generation of a dipole of edge dislocations with Burgers vectors ±**s** at crystal–glass interfaces A and B due to local shear events (ellipses) within the boundary region. (c) Further plastic shear in the amorphous boundary region results in increase of dislocation Burgers vectors up to $\pm\mathbf{b}_a$. (d) Splitting of one of the dislocations of the dipole results in formation of both a residual immobile dislocation and a mobile partial dislocation that glides in grain IV. The glide of the partial dislocation is accompanied by formation of stacking fault (wavy line). Magnified insets (a)–(d) illustrate evolution of the dislocation structure at the crystal–glass interface B. Reproduced from [33] with permission. Copyright (2006), Elsevier.

(GBDs) as well as experimentally observed effect of GB bowing (Fig. 2). Through energetic description, both processes were found to be highly sensitive to applied mechanical stress and GB misorientation angle. The results of this theoretical model account for experimental observations of curved GBs [16] and emission of partial dislocations by GBs [16] in deformed NC metals.

Gutkin and Ovid'ko [7] developed theoretical description of the generation of rectangular lattice perfect, lattice partial and GB dislocation loops at similar pre-existent dislocation loops and showed that these modes of dislocation generation can effectively provide plastic flow transfer from grain to grain, from grain to GB, from GB to grain, and from GB to GB in deformed NCMs, depending on their geometric and material characteristics. Bobylev et al. [8,9] further developed this approach and considered more general case of the generation of two (one after another) rectangular lattice partial dislocation loops at a pre-existent GB dislocation loop (Fig. 3) with these two new loops having arbitrary Burgers vectors making the gliding segments of the loops of either mixed (edge and screw) or screw types (before they were of the edge type only [7]). Three different dislocation slip systems typical for the face-centered cubic (FCC) crystalline lattice were considered and it was found that emission of the partial dislocation loops belonging to the 60°-I slip system is the most probable in nanocrystalline FCC metals. This model also allowed to establish that experimentally detected [18] anomalously wide stacking faults in nanocrystalline Al are caused by high stresses but not by small grain size as was initially believed [18,31 32].

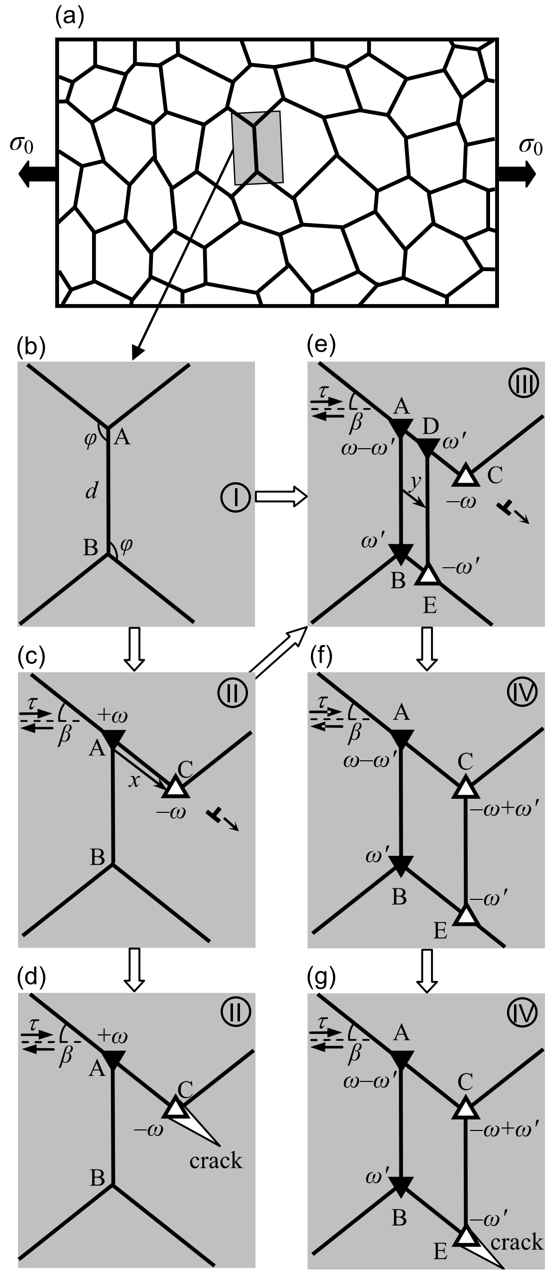

Fig. 5. GB sliding, splitting and migration processes in NC. (a) General view. (b) Initial configuration I of GBs is presented. (c) Configuration II results from "pure" GB sliding that produces a dipole of wedge disclinations A and C (small triangles). (d) Crack forms at the disclination dipole AC and grows into the grain interior. (e) Configuration III results from the cooperative GB sliding and nanograin nucleation process. GB AB splits into immobile grain boundary (also called AB) and mobile GB DE. The mobile boundary DE migrates under the shear stress and carries nanoscale plastic flow. (f) When the disclinations D and E converge, the configuration IV forms, which contains the two disclination dipoles. (g) Crack forms at the disclination dipole BE and grows along a grain boundary fragment. Reproduced from [41] with permission. Copyright (2011), The American Physical Society.

In a similar manner, Bobylev et al. [33] considered the generation of lattice partial dislocations at amorphous GBs in NC ceramics. Within the framework of the model, a dipole of immobile non-crystallographic edge dislocations is generated at the triple junctions (at the ends of an amorphous GB) through local shear events in this GB (Fig. 4). These dislocations can split resulting in emission of partial lattice dislocations into grain interior. It was concluded that this process is energetically favorable and can proceed in athermal way in nanocrystalline 3C–SiC. The critical stress required to carry out this process was found to decrease with an increase of the GB length (in fact, the grain size). In other words, the transition from intergranular slip to intragranular dislocation slip becomes more difficult as the grain size decreases.

4. GRAIN BOUNDARY SLIDING AND MECHANISMS OF ITS ACCOMMODATION

Among the modes of GB mediated plastic deformation, one of the key mechanisms is GB sliding. In particular, it has been experimentally proven that GB sliding processes dominate during superplastic deformation of NC metals [2]. Computer simulations [34,35] also confirm the key role of GB sliding in plastic deformation of NC metals, especially at high stresses and strain rates [36]. GB sliding is plastic shears localized within GBs and normally it creates defects – sources of internal stresses – in GB triple junctions capable of initiating the nucleation of nanocracks and subsequent brittle fracture of the nanomaterial [2,12]. However, in the material, in parallel with GB sliding, accommodation processes can develop, which transform defects produced by GB sliding severely reducing the level of internal stresses and increasing ductility and fracture toughness of the nanomaterial. Understanding the micromechanics of these accommodation processes provides key insight in the nature of superplastic deformation of NCMs.

Typical GB sliding accommodation mechanisms include the emission of lattice dislocations from GB triple junctions [27–29], diffusion [37,38], and rotational deformation [39]. At the same time, some original approaches have been developed in our lab like accommodation via GB splitting and migration [40,41]. In particular, Bobylev et al. [41] developed a theoretical model of the mechanism of cooperative action of GB sliding, GB splitting and GB migration (Fig. 5), which plays the role of a special mode of plastic deformation in NC metals. It was shown that GB sliding and GB migration are able to effectively accommodate each other by transforming GB disclinations. It was shown theoretically (using nanocrystalline Ni as an example) that the ductility and

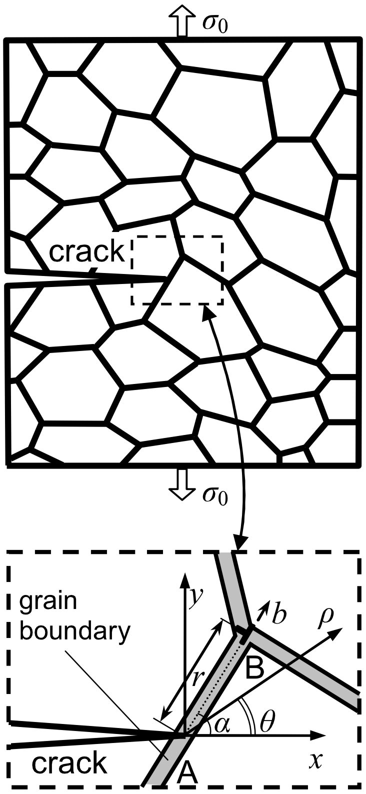

Fig. 6. Crack in a deformed nanocrystalline solid. The magnified inset highlights generation of an edge dislocation at the boundary (GB or amorphous intergranular boundary) near the tip of a long crack that intersects the boundary. Reproduced from [37] with permission. Copyright (2010), Elsevier.

fracture toughness of a material increases if the described cooperative mechanism dominates over pure GB sliding or cooperative GB sliding and migration (without GB splitting [40]). The results of theoretical analysis (in particular, the formation of nanograins in the vicinity of GB triple junctions) are consistent with experimental data [42,43] and computer models [44,45] on the observation of nano- and microscopic grain nucleation at triple junctions.

Accommodation of GB sliding affects not only ductility, but fracture toughness as well. Bobylev et al. [37] investigated fracture toughness enhancement by means of non-accommodated and accommodated GB sliding in NCMs at low and medium temperatures, respectively. In the case of non-accommodated GB sliding, immobile non-crystallographic Volterra dislocations are produced at GB triple junctions near crack tips at relatively low temperatures (Fig. 6). For nanocrystalline Al, Ni, and 3C–SiC, using the force criterion of crack growth, it was calculated that the effective stress intensity factor K^*_{IC} (fracture toughness) increases by up to 30% due to the dislocation created by non-accomodated GB sliding. The effect is stronger when dislocation is closer to the triple junction. The sensitivity of the stress intensity factor to this distance correlates with the sensitivity to grain size, since the smaller the grain size, the greater the probability of detecting a triple junction near the crack tip. At higher temperatures, GB sliding is effectively accommodated by diffusion-controlled climb of GBDs (Fig. 7) and emission of lattice dislocations into the grain body. Accommodated GB sliding can lead to significant blunting of crack tips, which, in turn, significantly (from 1.1 to 3 times, depending on temperature) increases fracture toughness. This effect is most pronounced in nanomaterials with very small grain sizes and decreases significantly with increasing grain size as K^*_{IC}~$d^{-5/2}$.

Bobylev et al. [39] considered a special mechanism of transition from GB sliding into rotational deformation in NCMs. This transition is also a mechanism for the accommodation of GB sliding. The mechanism was effectively described through the formation of immobile wedge disclinations at GB triple junctions characterized by gradually increasing power ω_0 in the stress field of two pile-ups of GBDs (Fig. 8). Calculations using Ni and α-Al_2O_3 as examples demonstrated that this mechanism is energetically favorable. Analytical expression for ω_0 (which is equilibrium disclination power equal to the angle of grain rotation) was obtained:

$$\omega_0 = \frac{2(\tau / D)qt - b\sum_{i=1}^{n} \ln \dfrac{(x_i - p)^2 + q^2}{(x_i + p)^2 + q^2}}{2q\left[(1+t^2)\ln(1+t^2) - t^2 \ln t^2\right]}, \qquad (1)$$

where D=G/[2π(1-ν)], G is the shear modulus, ν is the Poisson ratio, b is the magnitude of GBD Burgers vector, q=p/q (see Fig. 8), x_i is the coordinates of GBD dislocations. Equilibrium disclination power was found to be in the range from 3° to 7.5° in nanocrystalline Ni when applied shear stress τ = 0.5 GPa, and from 4° to 11° in nanocrystalline α-Al_2O_3 when τ = 2 GPa.

5. GRAIN BOUNDARY MIGRATION AND DEFORMATION-INDUCED GRAIN GROWTH AND REFINEMENT

Ultrafine-grained (UFG) and NC structures are typically formed due to severe plastic deformation that causes grain refinement in initially coarse-grained structures. In order to control the final UFG and NC structures in severely deformed materials, it is important to understand and describe both the nature and micromechanisms of deformation-induced grain refinement. In these circumstances, of particular interest is the stress-driven GB migration which by definition represents a plastic deformation mode carried by migrating GBs [13]. It is conventionally treated that the stress-

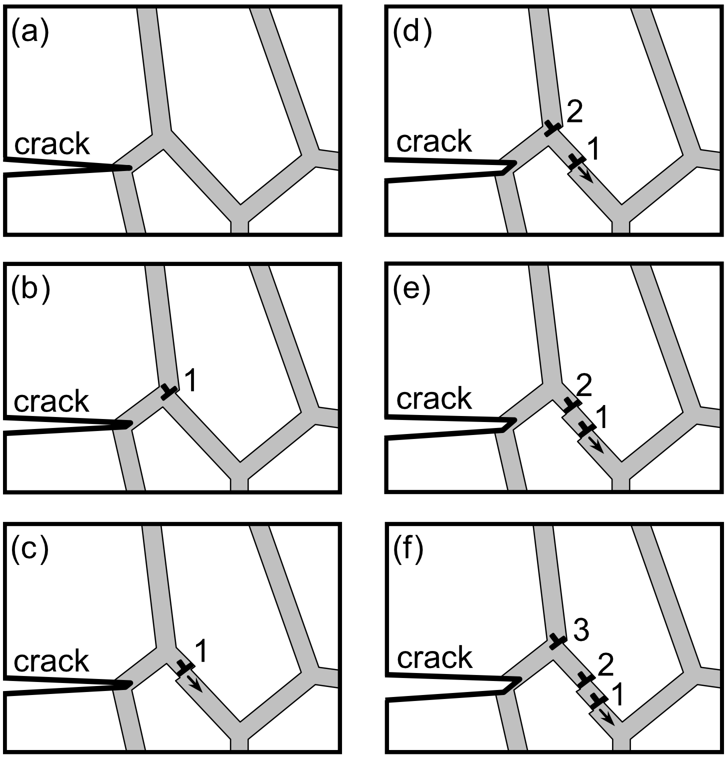

Fig. 7. GB sliding is accommodated through climb of grain boundary dislocations. Intergrain sliding near a crack tip produces triple junction dislocations. These dislocations climb away, in which case intergrain sliding is enhanced and leads to the blunting of the crack. Reproduced from [37] with permission. Copyright (2010), Elsevier.

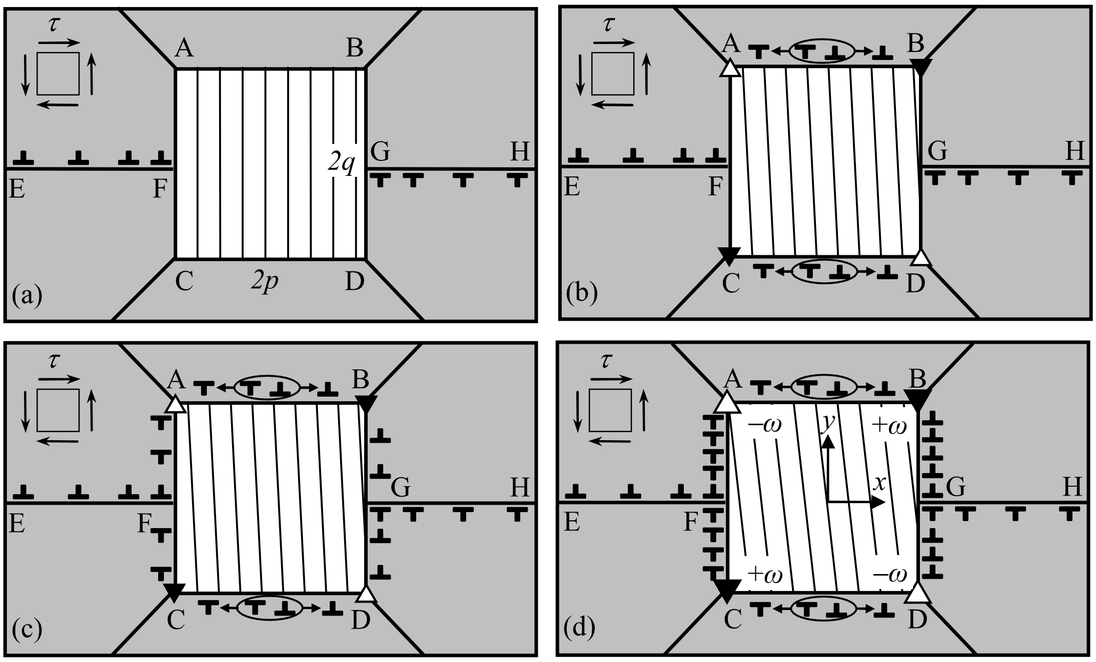

Fig. 8. Model of rotation deformation initiated by GB sliding. (a) Initial structure containing a rectangular grain ABCD. Two pile-ups of grain boundary dislocations are formed at segments EF and GH of mesoscopic sliding surface. (b) New grain boundary dislocations are generated at horizontal grain boundaries AC and BD under the action of the external shear stress and the stress fields of the pile-ups of grain boundary dislocations. (c) and (d) Special rotation deformation occurs in a nanograin through formation of immobile disclinations (triangles) whose strengths gradually increase during the formation process conducted by grain boundary dislocation slip and climb. In the situation (d), the system reaches its dynamic equilibrium state in which the dislocation generation at the horizontal grain boundaries AB and CD as well as within the mesoscopic sliding surface segments EF and GH is completely compensated by the dislocation annihilation at the triple junctions F and G.

driven GB migration is responsible for both nanoscale plastic flow and grain growth [13].

A brief summary of early experimental observations of athermal stress-driven grain growth and GB migration is given in [46]. Gutkin and Ovid'ko [47] suggested probably the first simple analytical model to describe this phenomenal. They treated the migration of a tilt GB, characterized be the length $2a$ and the misorientation angle ω, over a distance d under an applied shear stress τ as an athermal process accompanied with generation of a quadrupole of partial wedge disclinations with strength ω and sizes $d \times 2a$. Analyzing the energy change caused by this process, they found two critical stress values: τ_{c1} which is necessary for starting the GB migration, and τ_{c2} which separate the stable and unstable regimes of the GB migration. These critical stresses are given by very simple formulas [46, 47]:

$$\tau_{c1} \approx \frac{D\omega b}{2a}\left(\ln\frac{2a}{b}+\frac{1}{2}\right), \quad \tau_{c2} \approx 0.8D\omega, \tag{2}$$

where $D=G/[2\pi(1-\nu)]$, G is the shear modulus, ν is the Poisson ratio, and b is the interatomic distance. It was also shown that, if $\tau_{c1} \leq \tau \leq \tau_{c2}$, the equilibrium distance d_{eq} of the GB migration is determined from the following equation:

$$\tau = \frac{D\omega\, d_{eq}}{2a}\ln\left(1+\frac{4a^2}{d_{eq}}\right). \tag{3}$$

If $\tau > \tau_{c2}$, the GB migration becomes unstable when the GB propagation does not depend on the value of τ. This model was later supported by computer simulations [48].

Alternative role of stress-driven GB migration as a process responsible for nucleation of new nano-grains in NC and UFG materials (deformation-induced grain refinement) has been suggested and investigated in a number of works [40,41,49–53]. The common approach employed in these works is a disclination description of stress-induced GB splitting and migration (modeled as splitting and movement of disclination dipoles) resulting in nucleation of new nanograins. First models using this method were developed by Bobylev and Ovid'ko [49,50]. Within the framework of these models, nanograin nucleation occurs through splitting and migration of GBs containing disclination dipoles produced by GB sliding and/or lattice slip (Fig. 5). It was shown that the nanograin nucleation is energetically favorable in mechanically loaded NC Al and α-Al_2O_3 in certain ranges of their parameters and the external stress levels.

Models [49,50] considered simplified GB migration scenario producing rectangular nanograins. More realistic hexagonal grain shapes were considered by Bobylev et al. [41] in a similar manner. Further development of this approach included description [51] of nanograin nucleation near crack tips in NCMs, where GB splitting happened at a highly stressed, disclination-free region near a crack tip. The suggested theoretical models [41,51] of plastic flow occurring through generation of nanograins at GBs in UFG materials were well consistent with the experimental observation [42] of nanograins generation at GBs in cobalt.

Bobylev and Ovid'ko [53] extended description above on deformation-distorted GBs — non-equilibrium GBs containing trapped ensembles of lattice dislocations (Fig. 9) typical for NC and UFG materials produced by severe plastic deformation methods. It was concluded that the splitting processes in deformation-distorted GBs is specific to these GBs and do not have their analogs in the previously examined conventional, non-distorted GBs and lead to formation of new nanoscale (sub)-grains in nanomaterials. Thus, the stress-driven splitting of deformation-distorted GBs can effectively contribute to grain refinement in bulk metallic materials under severe plastic deformation.

Common feature of GB migration processes is the existence of unstable migration regime [45–53] and corresponding critical stress τ_{c2} for its onset. When applied stress exceeds this critical stress, GB starts migrating uncontrollably until it is stopped at some obstacle or destroyed completely (which is the case with low-

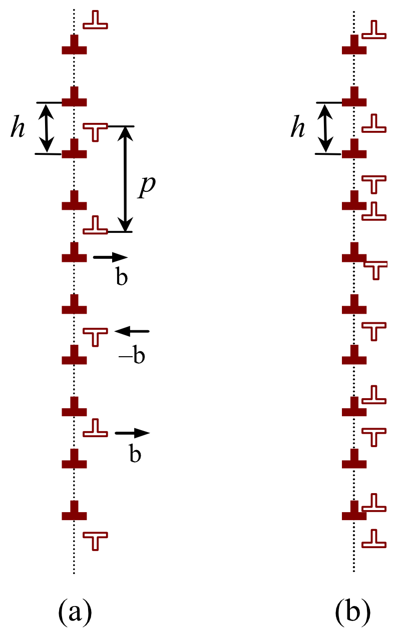

Fig. 9. Dislocation structures of deformation-distorted low-angle tilt boundaries. Each deformation-distorted low-angle grain boundary is represented as a dislocation wall consisting of both equilibrium (solid dislocation signs) and non-equilibrium (open dislocation signs) lattice edge dislocations. They can be arranged either (a) periodically or (b) randomly. Reproduced from [53] with permission. Copyright (2015), Elsevier.

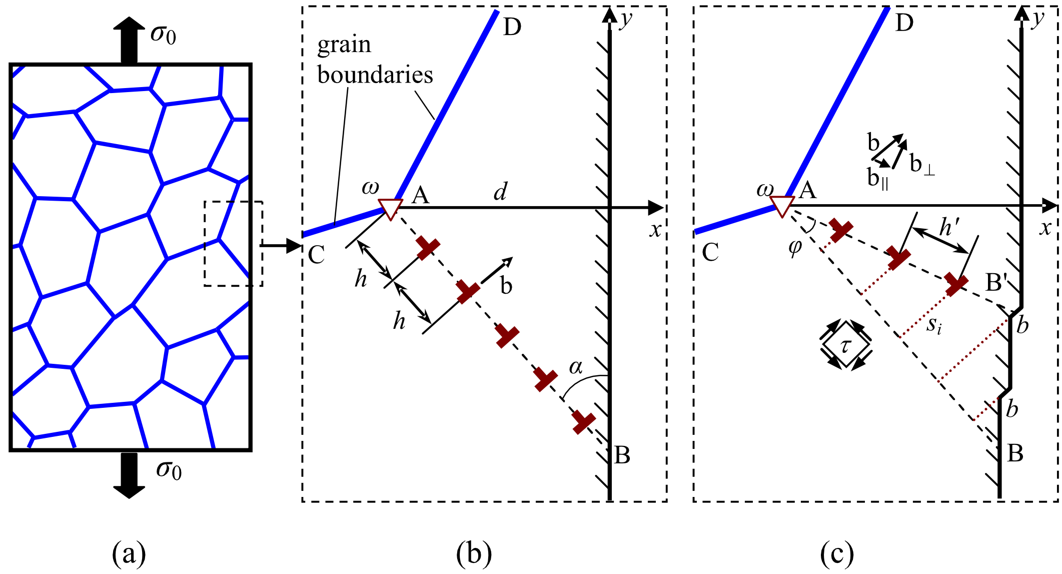

Fig. 10. GB rotation near free surface. (a) General view of nanocrystalline specimen. (b),(c) Magnified inset of the subsurface region where stress-driven rotation of a tilt grain boundary occurs. (b) Initial state. A low-angle symmetric tilt boundary AB is located near the free surface and forms a triple junction A with two static symmetric tilt boundaries AC and AD. (c) Stress-driven cooperative motion of GBDs occurs which results in tilt boundary rotation (by angle j) from its initial location AB to a new location AB'. Also, grain boundary rotation leads to the disappearance of several grain boundary dislocations at the free surface and associated formation of free-surface steps. Reproduced from [60] with permission. Copyright (2012), The American Physical Society.

angle GBs). Bobylev and Ovid'ko [53,54] assumed that this process is effectively controls grain refinement under SPD processing. It is known [55] that the grain size of metallic materials processed by SPD cannot be reduced below certain minimum value, i.e. there exists saturation of grain size. Indeed, grain refinement often occurs through formation and evolution of lattice dislocation cells [56]. In their turn, individual dislocations that form cell boundaries are generated at sources like Frank-Read ones. Thus, Bobylev and Ovid'ko [53,54] assumed that saturation of grain size in metals under SPD occurs when the dislocation cell boundaries start intensively migrating (in unstable regime). Saturated grain size can then be estimated via the balance of the critical stress τ_{c2} and the stress of Frank-Read source operation. The following estimation for saturated grain size d_s was obtained:

$$d_s \approx \frac{15\pi(1-\nu)b}{2\omega}. \quad (4)$$

Using Eq. (5) in the case of dislocation cell misorientation ~1°–3°, Bobylev and Ovid'ko [53,54] estimated d_s~78 - 233 nm in Cu and ~ 80 - 239 nm in Ni. These estimates are well consistent with experiments showing d_s ~ 200 nm in Cu processed by equal-channel angular pressing [57], and d_s ~ 50 - 200 nm in Ni processed by high pressure torsion [58,59].

Bobylev and Ovid'ko [60] suggested a new physical mechanism of plastic flow – GB rotations near free surfaces that can effectively occur in NC and conventional solids. A low-angle tilt boundary rotates through stress-driven cooperative motion of its constituent edge dislocations and results in transformation of the GB structure (Fig. 10). They demonstrated that the GB rotation is an energetically favorable process in NC nickel at high stresses in wide ranges of GB parameters. The suggested representations of GB rotation as a new deformation mode in solids are very consistent with the experimental observation [61] of GB rotations in deformed NC nickel nanopillars with grain size of around 60 nm. Similar description [62] was later suggested for high-angle GBs.

6. CONCLUSIONS

Thus we briefly reviewed theoretical models describing various aspects of GB transformations realized in plastically deformed NCMs. These models demonstrate that GBs play extensive role in deformation process and can affect it in a number of different ways. We have shown that GBs can serve as an alternative source of mobile lattice dislocations making standard intragranular dislocation slip viable mechanism in NCMs (until grain size becomes extremely small). Various transformation of GB structures such as the emission of lattice dislocations from GB triple junctions, GB diffusion, GB migration, GB splitting and rotational deformation can effectively accommodate GB sliding providing key insight into the nature of superplastic behaviour and fracture toughness enhancement of NCMs. Also it was shown that stress-induced GB migration can govern both deformation-induced grain growth and grain refinement.

In conclusion, we should note that present review covers only the matter of GB related mechanisms, while in NCMs plastic deformation develops through simultaneous action of various interacting physical mechanisms involving all elements of the defect structure, both in the bulk of nanograins and in their boundaries and triple junctions. Thus, proper theoretical description of the plastic deformation in NCMs must include all manner of existing structural elements.

REFERENCES

[1] S.V. Bobylev and I.A. Ovid'ko, *Granitsy zeren i plasticheskaya deformatsiya v nanomaterialah (Grain boundaries and plastic deformation in nanomaterials),* Izd-vo Polytechn. un-ta, Saint-Petersburg, 2016.

[2] M.Yu. Gutkin and I.A. Ovid'ko, *Defekty i mehanizmy plastichnosti v nanostrukturnyh i nekristallicheskih materialah (Defects and mechanisms of plasticity in nanostructured and non-crystalline materials),* Yanus, Saint-Petersburg, 2001.

[3] C.C. Koch, I.A. Ovid'ko, S. Seal and S. Veprek, *Structural nanocrystalline materials: fundamentals and applications,* Cambridge University Press, Cambridge, 2007.

[4] S.V. Bobylev, M.Yu. Gutkin and I.A. Ovid'ko, *Decay of low-angle tilt boundaries in deformed nanocrystalline materials,* J. Phys. D: Appl. Phys., 2004, vol. 37, no. 2, pp. 269–272. https://doi.org/10.1088/0022-3727/37/2/016

[5] S.V. Bobylev, M.Yu. Gutkin and I.A. Ovid'ko, *Chain decay of low-angle tilt boundaries in nanocrystalline materials,* Phys. Sol. State, 2004, vol. 46, pp. 2053–2057. https://doi.org/10.1134/1.1825548

[6] S.V. Bobylev, M.Yu. Gutkin and I.A. Ovid'ko, *Transformations of grain boundaries in deformed nanocrystalline materials,* Acta Mater., 2004, vol. 52, no. 13, pp. 3793–3805. https://doi.org/10.1016/j.actamat.2004.04.029

[7] M.Yu. Gutkin and I.A. Ovid'ko, *Generation of dislocation loops in deformed nanocrystalline materials,* Phil. Mag., 2006, vol. 86, no. 11, pp. 1483–1511. https://doi.org/10.1080/14786430500199302

[8] S.V. Bobylev, M.Yu. Gutkin and I.A. Ovid'ko, *Partial and split dislocation configurations in nanocrystalline metals,* Phys. Rev. B, 2006, vol. 73, no. 6, art. 064102. https://doi.org/10.1103/PhysRevB.73.064102

[9] S.V. Bobylev, M.Yu. Gutkin and I.A. Ovid'ko, *Generation of glide split-dislocation half-loops by grain boundaries in nanocrystalline Al,* Phys. Sol. State, 2006, vol. 48, no. 8, pp. 1495–1505. https://doi.org/10.1134/S1063783406080130

[10] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Generation of deformation twins in nanocrystalline metals: theoretical model.* Phys. Rev. B, 2006, vol. 74, no. 17, art. 172107. https://doi.org/10.1103/PhysRevB.74.172107

[11] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Mechanism of deformation-twin formation in nanocrystalline metals,* Phys. Sol. State, 2007, vol. 49, pp. 874–882. https://doi.org/10.1134/S1063783407050125

[12] N.F. Morozov, I.A. Ovid'ko, Yu.V. Petrov and A.G. Sheinerman, *Generation and convergence of nanocracks in nanocrystalline materials deformed by grain boundary sliding,* Rev. Adv. Mater. Sci., 2009, vol. 19, no. 1/2, pp. 63–72. https://www.ipme.ru/e-journals/RAMS/no_11909/morozov.pdf

[13] T.J. Rupert, D.S. Gianola, Y. Gan and K.J. Hemker, *Experimental observations of stress-driven grain boundary migration*, Science, 2009, vol. 326, no. 5960, pp. 1686–1690. https://doi.org/10.1126/science.1178226

[14] X.L. Wu and E. Ma, *Dislocations in nanocrystalline grains,* Appl. Phys. Lett., 2006, vol. 88, no. 23, art. 231911. https://doi.org/10.1063/1.2210295

[15] X.L. Wu and E. Ma, *Accommodation of large plastic strains and defect accumulation in nanocrystalline Ni grains,* J. Mater. Res., 2007, vol. 22, no. 8, pp. 2241–2253. https://doi.org/10.1557/jmr.2007.0279

[16] X.Z. Liao, F. Zhou, E.J. Lavernia, S.G. Srinivasan, M.I. Baskes, D.W. He and Y.T. Zhu, *Deformation mechanism in nanocrystalline Al: Partial dislocation slip,* Appl. Phys. Lett., 2003, vol. 83, no. 4, pp. 632–634. https://doi.org/10.1063/1.1594836

[17] X. Wu, Y.T. Zhu, M.W. Chen and E. Ma, *Twinning and stacking fault formation during tensile deformation of nanocrystalline Ni,* Scr. Mater., 2006, vol. 54, no. 9, pp. 1685–1690. https://doi.org/10.1016/j.scriptamat.2005.12.045

[18] Y.T. Zhu, X.L. Wu, X.Z. Liao, J. Narayan, S.N. Mathaudhu and L.J. Kecskés, *Twinning partial multiplication at grain boundary in nanocrystalline fcc metals,* Appl. Phys. Lett.,

2009, vol. 95, no. 3, art. 031909. https://doi.org/10.1063/1.3187539

[19] Y.M. Wang, E.M. Bringa, J.M. McNaney, M. Victoria, A. Caro, A.M. Hodge, R. Smith, B. Torralva, B.A. Remington, C.A. Schuh, H. Jamarkani and M.A. Meyers, *Deforming nanocrystalline nickel at ultrahigh strain rates*, Appl. Phys. Lett., 2006, vol. 88, no. 6, art. 061917. https://doi.org/10.1063/1.2173257

[20] V. Yamakov, D. Wolf, S.R. Phillpot and H. Gleiter, *Deformation twinning in nanocrystalline Al by molecular-dynamics simulation*, Acta Mater., 2002, vol. 50, no. 20, pp. 5005–5020. https://doi.org/10.1016/S1359-6454(02)00318-X

[21] H. Van Swygenhoven, *Footprints of plastic deformation in nanocrystalline metals*, Mater. Sci. Eng. A, 2008, vol. 483–484, pp. 33–39. https://doi.org/10.1016/j.msea.2006.10.204

[22] M.Yu. Gutkin, A.L. Kolesnikova, I.A. Ovid'ko and N.V. Skiba, *Rotational deformation in fine-grained materials prepared by severe plastic deformation*, J. Metastab. Nanocryst., 2002, vol. 12, pp. 47–57. https://doi.org/10.4028/www.scientific.net/JMNM.12.47

[23] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Changes in the grain boundary misorientation caused by emission of dislocation pairs*,Tech. Phys. Letters, 2002, vol. 28, pp. 437–438. https://doi.org/10.1134/1.1482760

[24] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Transformations of grain boundaries due to disclination motion and emission of dislocation pairs*, Mater. Sci. Eng. A, 2003, vol. 339, no. 1–2, pp. 73–80. https://doi.org/10.1016/S0921-5093(02)00107-7

[25] M.Yu. Gutkin, A.L. Kolesnikova, I.A. Ovid'ko and N.V. Skiba, *Disclinations and rotational deformation in fine-grained materials*, Phil. Mag. Lett., 2002, vol. 82, no. 12, pp. 651–657. https://doi.org/10.1080/0950083021000036742

[26] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Emission of partial dislocations by grain boundaries in nanocrystalline metals*, Phys. Sol. State, 2004, vol. 46, 2042–2052. https://doi.org/10.1134/1.1825547

[27] A.A. Fedorov, M.Yu. Gutkin and I.A. Ovid'ko, *Transformations of grain boundary dislocation pile-ups in nano- and polycrystalline materials*, Acta Mater., 2003, vol. 51, no. 4, pp. 887–898. https://doi.org/10.1016/S1359-6454(02)00433-0

[28] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Emission of partial dislocations from triple junctions of grain boundaries in nanocrystalline materials*, J. Phys. D: Appl. Phys., 2005, vol. 38, no. 21, pp. 3921–3925. https://doi.org/10.1088/0022-3727/38/21/013

[29] M.Yu. Gutkin, I.A. Ovid'ko and N.V. Skiba, *Grain boundary sliding and lattice dislocation emission in nanocrystalline materials under plastic deformation*, Phys. Sol. State, 2005, vol. 47, pp. 1662–1674. https://doi.org/10.1134/1.2045349

[30] Q. Wei, D. Jia, K.T. Ramesh and E. Ma, *Evolution and microstructure of shear bands in nanostructured Fe*, Appl. Phys. Lett., 2002, vol. 81, no. 7, pp. 1240–1242. https://doi.org/10.1063/1.1501158

[31] S.V. Bobylev and I.A. Ovid'ko, *Partial and split dislocations in deformed nanocrystalline metals*, Rev. Adv. Mater. Sci., 2004, vol. 7, no. 2, pp. 75–82. https://www.ipme.ru/e-journals/RAMS/no_2704/bobylev/bobylev.pdf

[32] Y.T. Zhu, X. Z. Liao, S.G. Srinivasan, Y.H. Zha, M.I. Baskes, F. Zhou, E.J. Lavernia, *Nucleation and growth of deformation twins in nanocrystalline aluminum*, Appl. Phys. Lett., 2004, vol. 85, no. 21, pp. 5049–5051. https://doi.org/10.1063/1.1823042

[33] S.V. Bobylev, A.K. Mukherjee and I.A. Ovid'ko, *Emission of partial dislocations from amorphous intergranular boundaries in deformed nanocrystalline ceramics*, Scr. Mater., 2009, vol. 60, no. 1, pp. 36–39. https://doi.org/10.1016/j.scriptamat.2008.08.025

[34] H. Van Swygenhoven and P.A. Derlet, *Grain-boundary sliding in nanocrystalline fcc metals*, Phys. Rev. B, 2001, vol. 64, no. 22, art. 224105. https://doi.org/10.1103/PhysRevB.64.224105

[35] J. Monk, B. Hyde and D. Farkas, *The role of partial grain boundary dislocations in grain boundary sliding and coupled grain boundary motion*, J. Mater. Sci., 2006, vol. 41, pp. 7741–7746. https://doi.org/10.1007/s10853-006-0552-3

[36] D. Wolf, V. Yamakov, S.R. Phillpot, A.K. Mukherjee and H. Gleiter, *Deformation of nanocrystalline materials by molecular-dynamics simulation: relationship to experiments?* Acta Mater., 2005, vol. 53, no. 1, pp. 1–40. https://doi.org/10.1016/j.actamat.2004.08.045

[37] S.V. Bobylev, A.K. Mukherjee, I.A. Ovid'ko and A.G. Sheinerman, *Effects of intergrain sliding on crack growth in nanocrystalline materials*, Int. J. Plasticity, 2010, vol. 26, no. 11, pp. 1629–1644. https://doi.org/10.1016/j.ijplas.2010.03.001

[38] I.A. Ovid'ko and A.G. Sheinerman, *Enhanced ductility of nanomaterials through optimization of grain boundary sliding and diffusion processes,* Acta Mater., 2009, vol. 57, no. 7, pp. 2217–2228. https://doi.org/10.1016/j.actamat.2009.01.030

[39] S.V. Bobylev, A.K. Mukherjee and I.A. Ovid'ko, *Transition from plastic shear into rotation deformation mode in nanocrystalline metals and ceramics,* Rev. Adv. Mater. Sci., 2009, vol. 19, no. 1/2, pp. 103–113. https://www.ipme.ru/e-journals/RAMS/no_11909/bobylev.pdf

[40] S.V. Bobylev, N.F. Morozov and I.A. Ovid'ko, I.A., *Cooperative grain boundary sliding and migration process in nanocrystalline solids,* Phys. Rev. Lett., 2010, vol. 105, no. 5, art. no. 055504. https://doi.org/10.1103/PhysRevLett.105.055504

[41] S.V. Bobylev, N.F. Morozov and I.A. Ovid'ko, I.A., *Cooperative grain boundary sliding and nanograin nucleation process in nanocrystalline, ultrafine-grained and polycrystalline solids,* Phys. Rev. B, 2011, vol. 84**, no. 9, art.** 094103. https://doi.org/10.1103/PhysRevB.84.094103

[42] X. Wu, N. Tao, Y. Hong, G. Liu, B. Xu, J. Lu and K. Lu, *Strain-induced grain refinement of cobalt during surface mechanical attrition treatment,* Acta Mater., 2005, vol. 53, no. 3, pp. 681–691. https://doi.org/10.1016/j.actamat.2004.10.021

[43] H. Miura, T. Sakai, S. Andiarwanto and J.J. Jonas, *Nucleation of dynamic recrystallization at triple junctions in polycrystalline copper,* Philos. Mag., 2005, vol. 85, no. 23, pp. 2653–2669. https://doi.org/10.1080/14786430500154257

[44] M.J. Demkowicz, A.S. Argon, D. Farkas and M. Frary, *Simulation of plasticity in nanocrystalline silicon,* Philos. Mag., 2007, vol. 87, no. 28, pp. 4253–4271. https://doi.org/10.1080/14786430701358715

[45] A. Cao and Y. Wei, *Atomistic simulations of crack nucleation and intergranular fracture in bulk nanocrystalline nickel,* Phys. Rev. B, 2007, vol. 76, no. 2, art. 024113. https://doi.org/10.1103/PhysRevB.76.024113

[46] M.Yu. Gutkin, K.N. Mikaelyan and I.A. Ovid'ko, Grain growth and collective migration of grain boundaries under plastic deformation of nanocrystalline materials. Phys. Solid State, 2008, vol. 50, pp. 1216–1229. https://doi.org/10.1134/S1063783408070135

[47] M.Yu. Gutkin and I.A. Ovid'ko, *Grain boundary migration as rotational deformation mode in nanocrystalline materials,* Appl. Phys. Lett., 2005, vol. 87, no. 25, art. 251916. https://doi.org/10.1063/1.2147721

[48] F. Sansoz and V. Dupont, *Grain growth behavior at absolute zero during nanocrystalline metal indentation*, Appl. Phys. Lett., 2006, vol. 89, no. 11, art. 111901. https://doi.org/10.1063/1.2352725

[49] S.V. Bobylev and I.A. Ovid'ko, *Nanograin nucleation initiated by intergrain sliding and/or lattice slip in nanomaterials,* Appl. Phys. Lett., 2008, vol. 92, no. 8, art. 081914. https://doi.org/10.1063/1.2885069

[50] S.V. Bobylev and I.A. Ovid'ko, *Nanograin nucleation through splitting and migration of grain boundaries in deformed nanomaterials,* Rev. Adv. Mater. Sci., 2008, vol. 17, no. 1/2, pp. 76–89. https://www.ipme.ru/e-journals/RAMS/no_11708/bobylev.pdf

[51] I.A. Ovid'ko, N.V. Skiba and A.K. Mukherjee, *Nucleation of nanograins near cracks in nanocrystalline materials,* Scr. Mater., 2010, vol. 62, pp. 387–390. https://doi.org/10.1016/j.scriptamat.2009.11.035

[52] N.F. Morozov, I.A. Ovid'ko and N.V. Skiba, *Stress-driven formation of nanograin chains in nanocrystalline and ultrafine-grained materials,* Rev. Adv. Mater. Sci., 2011, vol. 29, no. 2, pp. 180–186. https://www.ipme.ru/e-journals/RAMS/no_22911/11_ovidko1.pdf

[53] S.V. Bobylev and I.A. Ovid'ko, *Stress-driven migration of deformation-distorted grain boundaries in nanomaterials,* Acta Mater., 2015, vol. 88, pp. 260–270. https://doi.org/10.1016/j.actamat.2015.01.052

[54] S.V. Bobylev and I.A. Ovid'ko, *On minimum grain size in ultrafine-grained materials and Gum-metals processed by severe plastic deformation,* Mater. Phys. Mech., 2016, vol. 29, no. 1, pp. 17–23. https://www.ipme.ru/e-journals/RAMS/no_22911/11_ovidko1.pdf

[55] R. Pippan, S. Scheriau, A. Taylor, M. Hafok, A. Hohenwarter and A. Bachmaier, *Saturation of fragmentation during severe plastic deformation, Ann. Rev. Mater. Res., 2010, vol.* **40, pp.** 319–343. https://doi.org/10.1146/annurev-matsci-070909-104445

[56] Y. Estrin and A. Vinogradov, *Extreme grain refinement by severe plastic deformation: a wealth of challenging science,* Acta Mater., 2013, vol. 61, no. 3, pp. 782–817. https://doi.org/10.1016/j.actamat.2012.10.038

[57] F. Dalla Torre, R. Lapovok, J. Sandlin, P.F. Thomson, C.H.J. Davies and E.V. Pereloma,

Microstructures and properties of copper processed by equal channel angular extrusion for 1–16 passes, Acta Mater., 2004, vol. 52, no. 16, pp. 4819–4832. https://doi.org/10.1016/j.actamat.2004.06.040

[58] H.W. Zhang, X. Huang and N. Hansen, *Evolution of microstructural parameters and flow stresses toward limits in nickel deformed to ultrahigh strains*, Acta Mater., 2008, vol. 56, no. 19, pp. 5451–5465. https://doi.org/10.1016/j.actamat.2008.07.040

[59] E. Schafler and R. Pippan, *Effect of thermal treatment on microstructure in high pressure torsion (HPT) deformed nickel,* Mater. Sci. Eng. A, 2004, vol. 387–389, pp. 799–804. https://doi.org/10.1016/j.msea.2004.01.112

[60] S.V. Bobylev and I.A. Ovid'ko, *Grain boundary rotations in solids,* Phys. Rev. Lett, 2012, vol. 109, no. 17, art. no. 175501. https://10.1103/PhysRevLett.109.175501

[61] D. Jang and J. R. Greer, *Size-induced weakening and grain boundary-assisted deformation in 60 nm grained Ni nanopillars,* Scr. Mater., 2011, vol. 64, no. 1, pp. 77–80. https://doi.org/10.1016/j.scriptamat.2010.09.010

[62] S.V. Bobylev and I.A. Ovid'ko, *Stress-driven rotations of deformation distorted-grain boundaries in nanocrystalline and ultrafine-grained materials,* Rev. Adv. Mater. Sci., 2015, vol. 41, no. 1/2, pp. 20–34. https://www.ipme.ru/e-journals/RAMS/no_14115/03_14115_ovidko.pdf