Localization of plastic deformation and mechanical twinning in dynamical channel angular pressing

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Abstract. We have performed numerical simulations for the early stages (till several tens of microseconds) of dynamical channel angular pressing (DCAP). New dislocation and twinning models have been used for description of the kinetics and dynamics of defect structures; these models are described in the paper. In DCAP of copper with the initial sample velocities ranging from 100m/s to 250m/s we have found that the shock wave propagation leads to appearance of microscopic shear bands, its growth and intersections. We suppose that it is the main mechanism of the nanocrystalline grain formation. Twinning takes place in DCAP and the volume fraction of twins can go up to 0.5. It can be supposed that the shear bands and twins formation at the early stages of DCAP leads to some special features of the microstructure, which differs these structures from the structures obtained after quasi-static ECAP processes.

Keywords: dynamical channel angular pressing, shear band, localization, mechanical twinning, dislocations, plasticity.

Introduction

Plastic deformation is non-uniform over the volume in many cases of dynamic loading of metals [1,2]. Macroscopic and microscopic strain localization can be distinguished. The macroscopic localization is visible to the naked eye and the corresponding structures have a characteristic size of several millimeters. Their shape is determined by the sample geometry and by the boundary conditions. The microscopic localization consists in formation of shear bands with a width of up to several hundreds of micrometers [1,2]. The microscopic localization is the result of the plastic flow instability and traditionally associated with non-uniformities of the temperature field in the course of straining, which leads to the local softening of the material. Recent investigations [3] demonstrate that any non-uniformity in dislocation density and the presence of stress concentrators can provoke plastic flow localization. Therefore, any initial non-uniform dislocation distribution inherent to real materials can lead to localization of plastic flow at high strain rates [4]. Numerical investigations show that random perturbations of the dislocation density distribution lead to formation of shear band systems during the propagation of the shock wave through the perturbed sample [4]. It appears in dispersion of the mass velocity at the shock front, which has been observed experimentally [5].

Formation of twin structures is another well known feature of high strain rate deformation of metals [6,7]. Mechanical twinning is a complex process consisting of nucleation of twins and their further rapid growth in length and width; detwinning process can also take place. Description of twinning is very hard in the frame of continuous media mechanics because of the complexity of this phenomenon [8]. Most of the existing models for kinetics and dynamics of twins have many fitted parameters and suffer from low universality. High strain rates usually are examined in shock loading of the material when the strain does not exceed 5% [2]. Meanwhile, in the past decade some processes have been developed, which are characterized by high strain rates simultaneously with severe plastic deformation of the material. One of them is the dynamic channel angular pressing (DCAP) [9] in which intense and high rate plastic straining leads to a considerable change of defect substructure of the material. The DCAP method has been investigated in a number of recent publications [10-14]. It is essentially analogous to the widely spread method of the equal channel angular pressing (ECAP) [15,16], but the slow forcing of the work piece through an angular die by hydraulically press [15] is replaced by its shooting from a gas gun with velocities ranging from 100 m/s to 300 m/s [14]. When the work piece passes through the angular die, intense plastic deformation with a strain rate of 10^3–10^5 s^{-1} occurs in the sample. The higher values of the strain rate as compared to those in the ECAP processes impart new features to the evolution of the defect structure of the metal and results in unique characteristics of the samples obtained using DCAP [10,13,17]. There are two main experimentally observed and practically important features of the resultant ultrafine grained (UFG) structure in the case of DCAP [13,17]: (i) the presence of fine grains with grain sizes less than 100 nm and (ii) high stability of the resultant fine grain structures preserving their properties for a long time. These features advantage the DCAP-produced structured materials in comparison with microstructures produced by ECAP and other methods of quasi-static loading; the reasons for such difference still remain disputable.

In this paper we propose a new structural model for mechanical twinning which is combined with the original model of dislocation kinetics and dynamics presented in Refs. [18,19,20]. Also we numerically investigate the DCAP process on the basis of these plasticity models and analyze the evolution of the defect substructure of the metal during dynamic straining. Special attention is paid to the localization of the plastic flow as a straining mechanism, which changes the strength of the material and leads to bimodal grain size distribution.

1. Mathematical model

The mathematical model consists of continuum mechanics equations supplemented by equations for the plastic strain rates and the defects kinetics, which describe two competitive mechanisms of plasticity – the dislocation slip and mechanical twinning. This approach is useful for the numerical description of high strain rate deformation processes [18-20]. The full stresses σ_{ik} can be composed from the spherical part $-P\cdot\delta_{ik}$ and the stress deviator S_{ik}, where p is the pressure and δ_{ik} is the Kronecker delta: $\sigma_{ik}=-P\cdot\delta_{ik}+S_{ik}$. The generalized Hooke law [21] can be written then as follows:

$$S_{ik}=2G\left[u_{ik}-\frac{1}{3}u_{ll}\cdot\delta_{ik}-w_{ik}\right], \tag{1}$$

where G is the shear modulus, u_{ik} is the total deformation induced by the macroscopic motion of the material, w_{ik} is the plastic deformation tensor; the Einstein summation convention is used here and further. The time derivative of tensor u_{ik} is determined by the material velocity υ_i:

$$\frac{du_{ik}}{dt}=\frac{1}{2}\left(\frac{\partial \upsilon_i}{\partial x_k}+\frac{\partial \upsilon_k}{\partial x_i}\right)+\frac{1}{2}\left\{u_{il}\left(\frac{\partial \upsilon_k}{\partial x_l}-\frac{\partial \upsilon_l}{\partial x_k}\right)+u_{lk}\left(\frac{\partial \upsilon_i}{\partial x_l}-\frac{\partial \upsilon_l}{\partial x_i}\right)\right\}, \tag{2}$$

where x_l is the coordinate. The first term in the right-hand part of Eq. (2) is the infinitesimal strain rate tensor. The last term in the right-hand part of Eq. (2) accounts for the change of the deformation tensor components in the laboratory coordinate system due to a material rotation [22], which is essential for two or threedimensional cases.

We assume that the dislocation slip and twin formation inside the grains fully determine the plasticity of the considered polycrystalline metals. Then the plastic deformation tensor has two independent parts: one of them is the deformation caused by the dislocations slip w_{ik}^D, another one is the deformation caused by the twinning process w_{ik}^{TW}. The total plastic deformation can be written as a sum:

$$w_{ik}=w_{ik}^D+w_{ik}^{TW}. \tag{3}$$

For complete description of the deformation processes one needs to define these two plastic deformation tensors and their evolution in time.

Dislocation plasticity

1.1 Dislocation kinetics

For determination of the dislocation density evolution one can write a kinetics equation in the following form [18,20]:

$$\frac{d\rho_D^\beta}{dt}=\frac{\eta}{\varepsilon_L}\left\{2Bc_t^2\left[\left(\frac{1}{\sqrt{1-\left(V_D^\beta/c_t\right)^2}}-1\right)+b\sigma_y\left|V_D^\beta\right|\right]\right\}-k_a b\left|V_D^\beta\right|\left(\rho_D^\beta\right)^2-\frac{\rho_D^\beta\left|V_D^\beta\right|}{d}. \tag{4}$$

Here the dislocation source (the first term in the Eq. (4)) has been obtained from energy considerations; $\eta=0.1$ is the portion of dissipated power, which is spent on generation of new defects; the energy $\varepsilon_L=8eV/b$ [23] is required for generation of new dislocations per unit length, k_α is a parameter of dislocation annihilation [24], V_D is the dislocation velocity, ρ_D is the dislocation scalar density, and d is average grain size of the material. The annihilation term (the second term in the Eq. (4)) was written similar to [24].

1.2 Dislocation dynamics

We describe the plasticity caused by dislocation slip using the model proposed in [18]. In crystalline metals dislocations can glide along limited numbers of slip planes, which is numerated by the index β. The equation for the plastic deformation caused by dislocation glide [25] can be written as:

$$\frac{dw_{ik}^D}{dt}=\frac{1}{2}\sum_\beta\left(b_i^\beta n_k^\beta+n_k^\beta b_i^\beta\right)V_D^\beta\ \rho_D^\beta+\frac{1}{2}\left\{w_{il}^D\left(\frac{\partial \upsilon_k}{\partial x_l}-\frac{\partial \upsilon_l}{\partial x_k}\right)+w_{lk}^D\left(\frac{\partial \upsilon_i}{\partial x_l}-\frac{\partial \upsilon_l}{\partial x_i}\right)\right\}, \tag{5}$$

where the last term in the right-hand part has the same sense as the corresponding term of the Eq. (2); b^β is the Burgers vector of dislocations, ρ_D^β is the scalar density of dislocations of the slip plane with index β, V_D^β is the dislocation velocity. The dislocations density and their velocity fully determine the plastic deformation of the coarse-grained crystals. The dislocation velocity can be defined from the movement equation [18-20]:

$$\frac{m_0}{\left(1-\left(V_D^\beta / c_t\right)^2\right)^{3/2}} \frac{dV_D^\beta}{dt} = \left(F_D^\beta - \frac{b^\beta \sigma_y}{2} \cdot \mathrm{sign}\left(F_D^\beta\right)\right) - \frac{BV_D^\beta}{\left(1-\left(V_D^\beta / c_t\right)^2\right)^{3/2}}. \qquad (6)$$

Here $F_D^\beta = S_{ik} b_i n_k$ is the Peatch-Koehler force, which acts on the unit length of dislocation line from the stress field S_{ik}; σ_y is the static yield stress of the material, which depends on the dislocation density, the grain size and the presence of different impurities [26]; m_0 is the dislocation field mass [25]; c_t is the transverse sound velocity. The multipliers $\left(1-\left(V_D^\beta / c_t\right)^2\right)^{-3/2}$ in Eq. (6) allow one to take into account the experimental fact that the dislocation velocity is always limited by the transverse sound velocity. The viscous friction coefficient B is temperature dependent [18,23]. Eq. (6) has demonstrated a good fit with the experimental data for over barrier dislocation gliding at the high rate deformation [18-20]

1.3 Shear band formation after the shock wave front

The proposed model has been used for numerical investigation of plastic flow localization [3]. Fig. 2 shows a picture of localization of plastic flow behind the shock wave front moving through a sample with randomly perturbed dislocation density. One can see the formation of shear bands inclined at 45° to the shock wave front. Similar results have been obtained for perturbation of grain size; any perturbation leads to non-uniformity.

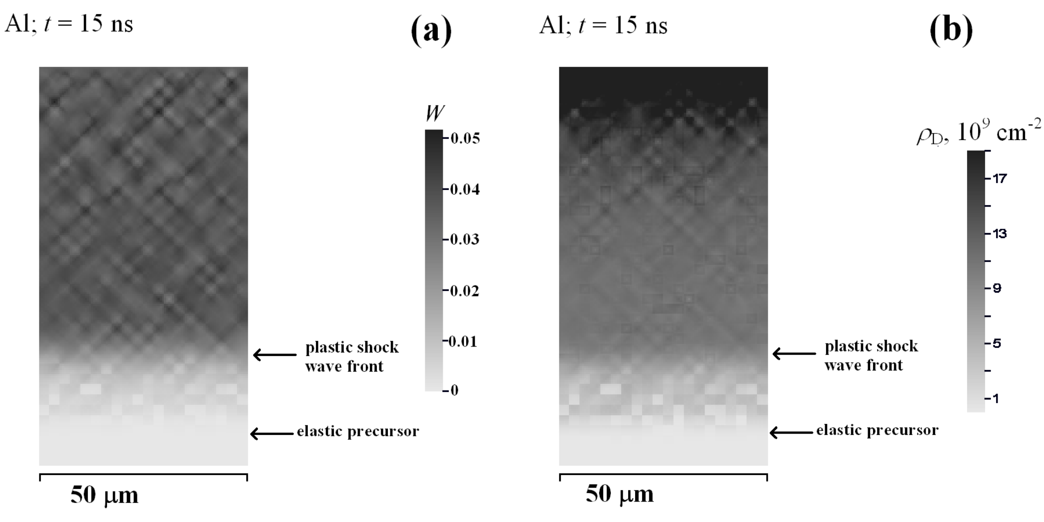

Figure 1
Localization of plastic flow on the shock wave front: the shock wave propagation in aluminium with randomly perturbed initial distribution of dislocation density; the

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plastic strain intensity (a) and the dislocation density (b). Formation of shear bands inclined at 45° to the shock wave front. The velocity jump in the shock wave is 0.3 km/s, it moves downwards.

1.4 Micro and macro localization of plastic flow at the initial stages of DCAP

The processes occurring during the first ten microseconds from the beginning of straining are of considerable interest for analysis of the features of generation and evolution of defect sub-structures. Calculations show that the instant of collision of the sample with the lower base of the angular die, at which a shock wave is formed and plastic strain localization bands are generated, is significant. It can be clearly seen that a shock wave of a particular shape propagates upwards in the sample, and the dislocation density in the metal considerably increases behind the wave front. The shock wave propagates in the sample during the first 10 μs of the straining process, which leads to an increase in the dislocation density from 10^8 to 10^{10} cm^{-2}. After the reflection from the upper free surface of the sample, the shock wave rapidly attenuates. This initial increase in the average dislocation density considerably distinguishes the DCAP method from the quasi-static ECAP method and must impart new features of the resultant defect structure of the material. As regards the non-uniformity of straining during DCAP, we can emphasize the macroscopic localization of the plastic flow, which is determined by the specific geometry of the angular die, and the microscopic localization of a more fundamental origin. The characteristic sizes of non-uniformities associated with the former mechanism are in the order of a millimeter.

As a result of DCAP, three macroscopic hardening bands can be distinguished in the metal; the strongest hardening is observed at the upper surface of the cylinder (region A in Fig. 2); the widest hardening band is located along the cylinder axis (region B), and its lower base is also hardened (region C). This is due to the fact that the strongest heating of the sample as a result of internal friction must occur in regions in which shear strains are maximal, and stress relaxation occurs due to dislocation slip leading to their intense accumulation in this region. Calculations show that the material is heated during DCAP only slightly, and temperature oscillations do not exceed 50 K. Thus, the macroscopic strain localization leads to non-uniform hardening of the material and to a non-uniform size distribution of grains over the sample, but must not change its mechanical properties significantly.

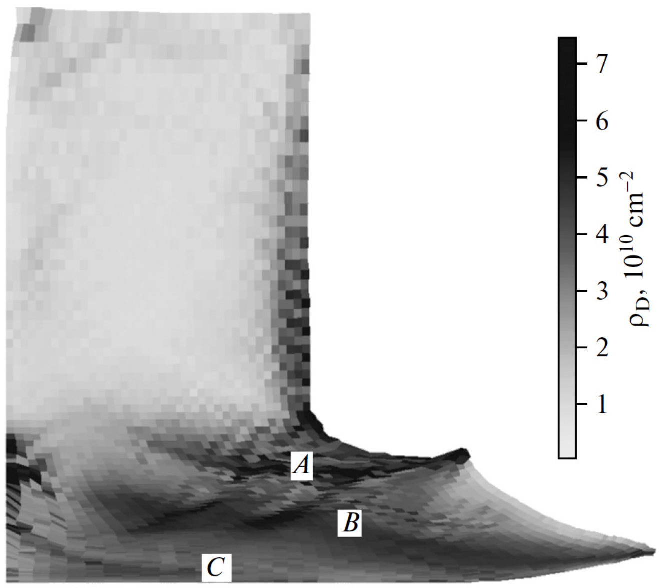


Figure 2
Dislocations distribution in the cross section of a copper cylinder (d = 5 mm, L = 16 mm) 25 μs after its collision with the base of the angular die at a velocity of V = 150 m/s [27].

The microscopic localization of the plastic flow in the shear bands is much more interesting for obtaining materials with special mechanical characteristics. This localization is almost independent of the form of macroscopic localization and generates a unique defect substructure in the material. Simulation results shown in Fig. 2 correspond to the results of calculations on a quite rough computational grid (100×50 meshes). On such a grid, the averaged characteristics of large volumes of the material are determined, which does not permit the observation of plastic flow localization associated with dislocation density fluctuations. To analyze the effects of microscopic localizations, we used a computational grid with 250×100 meshes, which allowed us to trace in detail the changes in the defect substructure of the material. Fig. 3 shows the results of simulations of DCAP of copper samples at instants of 4.5 and 9.5 μs after collision. We can see the evolution of the localized plasticity bands during the propagation of the shock wave, which are generated in the sample during collision. As in the calculations depicted in Fig. 2, the average dislocation density in the material increases from 10^8 to 10^{10} cm^{-2} as a result of passage of a shock wave through the sample. Individual vertical bands with a width of about 100 μm can be distinguished in which the dislocation density is almost an order of magnitude higher than in the surrounding material and attains a value of 7.5×10^{10} cm^{-2}. When the shock wave front reaches the upper boundary of the horizontal channel (about 16 mm from the die base), the localization band expands and generates a large number of localized plasticity bands oriented at an angle of 45° to the initial band (see Fig. 3). Such an unstable behavior of the band can be explained by the fact that the maximum shear stresses in the material are oriented precisely at this angle to the direction of propagation of the shock wave and by the effect of stresses localized at the joint between the vertical and horizontal channels of the angular die. It is also interesting to note that a thin layer with a lower density of defects is formed around the bands (see the inset to Fig. 3). Upon further propagation of the shock wave, the microscopic localization becomes less pronounced. Pair-wise intersection of the bands with elevated dislocation density must lead to the formation of a network of dislocation cells (see Fig. 3) with a dislocation density exceeding 10^{11} cm^{-2} in the regions of intersection. The repeated passage of the sample through the angular die must lead to the formation of grains with a size smaller than 80 nm, which were found after DCAP and were not observed in the structures obtained by quasi-static straining methods.

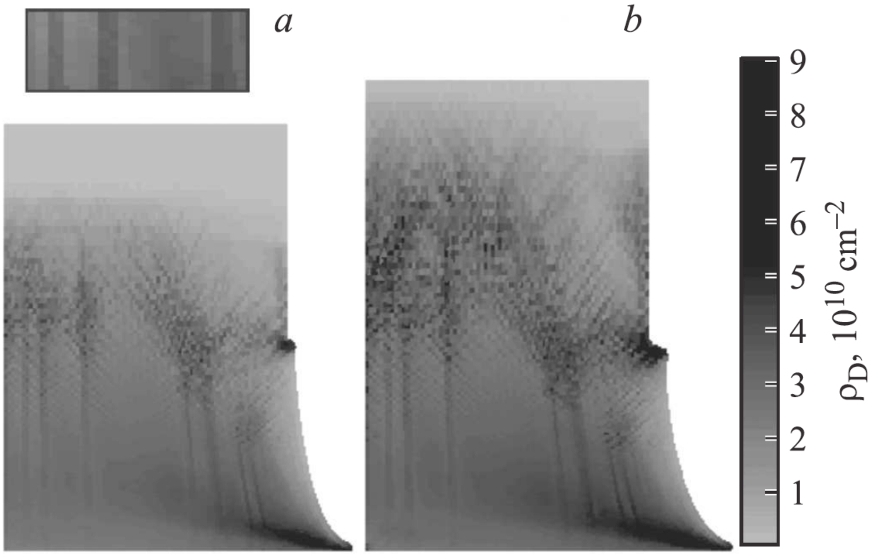


Figure 3
Microscopic plastic flow localization bands at instants of 4.5 μs (a) and 9.5 μs (b) [27]. An analogous pattern is observed for the temperature distribution over the sample cross section. The intersection of the localization bands can be seen. The inset shows the enlarged fragment near the base of the angular die, where regions with a lower dislocation density can be distinguished.

2. Model for mechanical twinning

2.1 Twinning kinetics

The above described dislocation plasticity model [1,2] is not enough at low temperatures or high strain rates because of the existence of mechanical twinning which is an alternative plasticity mechanism [1,2,6-8]. The main parameter which represents the twinability of the material is the stacking fault energy γ_{SF}. Twinning occurs if γ_{SF} of the metal is less than 100 mJ/m² which is the case for copper, steel and for many alloys. The generation of a twin can be described as an appearance of a stacking fault with size more than some critical value and its growth as a cooperative movement of partial dislocation outside the stacking fault [28].

Let us define N_{TW} as the number of growing twins per unit volume. We suppose that twinning takes place when the ordinary channel of stress relaxation due to dislocation gliding is suppressed. If dislocation, stored in the material, intensively annihilate with each other, than a part of the plastic deformation energy (elastic energy stored in the dislocation nuclei) dissipates [23] and cannot provide an effective stress relaxation. Therefore, it can be supposed, that this part of energy should be spent on twin nucleation as a more effective mechanism of stress relaxation. The twin nucleation rate can be expressed through the energy released by dislocation annihilation $\dot{N}_{TW}^{+} = \left(\varepsilon_D \dot{\rho}_D^{anh}\right) / \left(4\pi R_0^2 \gamma_{SF}\right)$, here $\dot{\rho}_D^{anh}$ is the rate of dislocation annihilation per unit volume, $\varepsilon_D \approx 8\,\mathrm{eV}/b$ is the elastic energy of dislocation per unit length [23], b is the length of the Burgers vector, R_0 is the size of the twin nucleus. The twin becomes immobilized when it grows up to another twin or grain boundary. The rate of twin immobilization can be written as $\dot{N}_{TW}^{-} = N_{TW}\left|\dot{R}\right|\left(\Delta^{-1} + d^{-1}\right)$, where $\dot{R}$ is the growth rate of the twin. The distance between twins Δ can be expressed through its volume fraction α_{TW} as $\Delta = h\left(1-\alpha_{TW}\right)/\alpha_{TW}$ [29], where h is the thickness of the twin. Then the nucleation rate of twins is: $\dot{N}_{TW} = \dot{N}_{TW}^{+} - \dot{N}_{TW}^{-}$, and finally:

$$\dot{N}_{TW} = \frac{\varepsilon_D \dot{\rho}_D^{anh}}{4\pi R_0^2 \gamma_{SF}} - N_{TW}\left|\dot{R}\right|\left(\frac{1}{\Delta} + \frac{1}{d}\right). \tag{7}$$

The dislocation annihilation rate per unit volume can be represented as follows [4,19]:

$$\dot{\rho}_D^{anh} = k_\alpha b\left|V_D\right|\rho_D^2 + \rho_D\left|V_D\right|/d, \tag{8}$$

where k_α is a parameter of dislocation annihilation [19], V_D is the dislocation velocity, and ρ_D is the dislocation scalar density.

2.2 Model of twin dynamics

After the nucleation of twin its continuous growth occurs through the moving of partial dislocations. They move under the action of elastic stress field and are slowed down by phonon dragging force. The surface energy of the growing twin continuously increases which leads to the appearance of an additional force. The shear deformation inside the twin for BCC and FCC metals [6] is equal to $\varepsilon_{TW} = 1/\sqrt{2}$. The forces acting along the radius and thickness of the twin can be obtained as:

$$\begin{aligned} F_R &= -\frac{\partial U}{\partial R} = 4\pi\varepsilon_{TW}\sigma_{ik}n_i\tau_k Rh - 2\pi\gamma_{SF}\left(2R+h\right) - \Phi Rh^2 \\ F_h &= -\frac{\partial U}{\partial h} = 2\pi\varepsilon_{TW}\sigma_{ik}n_i\tau_k R^2 - 2\pi\gamma_{SF}R - 2\Phi Rh \end{aligned} \tag{9}$$

here Φ is the elastic deformation energy of the lattice around the twin [30]:

$$\Phi = \frac{2\pi^2}{3}\frac{(2-\nu)}{(1-\nu)}G\varepsilon_{TW}^2 \tag{10}$$

These forces lead to twin growth both in length and thickness but simultaneously increase the twin surface energy which works against this growth. The phonon dragging force acts on a gliding partial dislocations resisting to the twin growth. Hence the condition of twin growth initiation is an excess of the external forces. It leads to an equation for twin length in the form:

$$\left(\frac{\dot{R}}{c_t}\right)^2 = \left(1-\left(\frac{\dot{R}}{c_t}\right)^2\right)^3\left(\frac{F_R}{c_t B_f^{part}}\right)^2. \tag{11}$$

Hereafter we designate with "*part*" parameters which correspond to partial dislocations inside the twins. If the twin boundary is fixed between the grains boundaries or other twins then only the thickness of twin can increase. It happens because partial dislocations glide along the twin boundaries. The twin thickness increases by the Burgers vector *b* at each act of the dislocation glide. The twin thickness increases with the rate of $\dot{h} = b/\left(V_D^{part} R\right)$. Therefore, the thickness growth rate is:

$$\left(\frac{R\dot{h}}{bc_t}\right)^2 = \left(1-\left(\frac{R\dot{h}}{bc_t}\right)^2\right)^3\left(\frac{F_h}{c_t B_f^{part}}\right)^2. \tag{12}$$

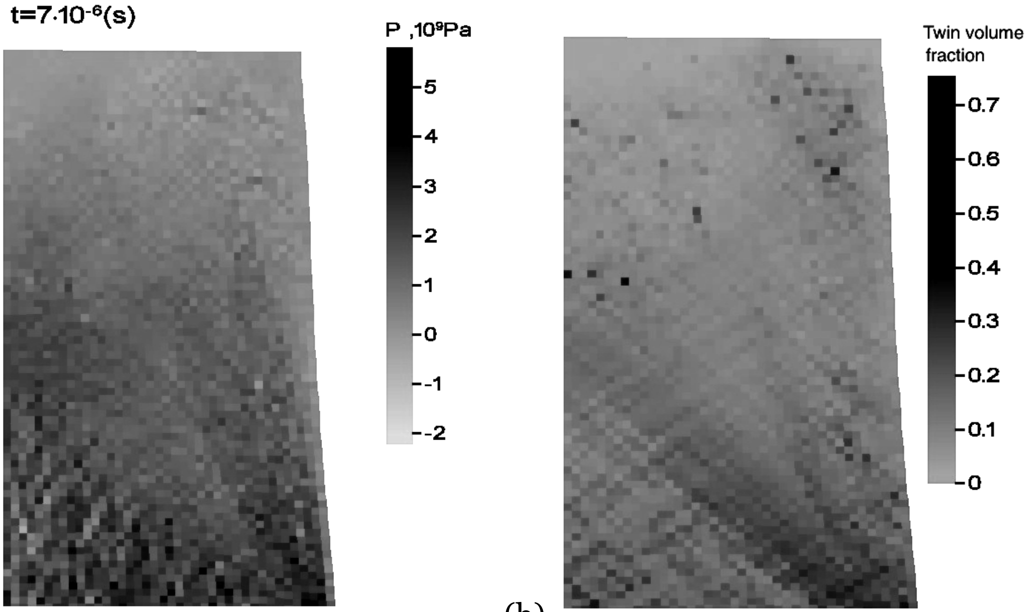
The strain rate is defined through volume fraction of twins α_{TW} as

$$\dot{w}_{ik}^{TW} = \sum_{\gamma}\dot{\alpha}^{\gamma}\left(n_i^{\gamma}\tau_k^{\gamma} + n_k^{\gamma}\tau_i^{\gamma}\right)\varepsilon_{TW} + \omega_{ik}^{TW} \tag{13}$$

where the summation is over all possible twinning planes numbered by the index γ. The rotation tensor ω_{ik}^{TW} is also taken into account [22].

2.3 Twins formation in DCAP process

The influence of twinning has been numerically estimated at the early stages of DCAP processing of a copper sample. Fig. 4 presents the simulation results by accounting of both the mechanical twinning and dislocation plasticity; the snapshot was taken at the time moment of 7 µs. High acting shear stresses (more than several GPa) lead to intensive twin nucleation and growth. The volume fraction of twins exceeds 0.6 for an initial velocity of the rod 150m/s; it is sufficient for considerable modification of the mechanical properties of the material.



(a) (b)

Figure 4

Stress distribution (a) and twin volume fraction (b) in copper rod in DCAP process. The initial rod geometry is: d = 5 mm, L = 16 mm, the velocity is 150m/s.

Conclusion

A new plasticity model has been described, which takes into account both dislocation plasticity and mechanical twinning. The model considers multiplication and gliding of dislocations, nucleation and growth of micro-twins as well as mutual influence of these defect subsystems. All possible crystallographic orientations of dislocations and twins were considered.

Simulations of DCAP were performed using the described mathematical models of dislocation plasticity and mechanical twinning. These simulations demonstrate the fundamental differences between quasi-static ECAP process and its dynamical modification, which is DCAP. The main reason of the differences is the presence of shock wave, which “prepares” the material before its severe deformation. The shock wave leads to plastic flow localization due to dislocation glide and to the intensive twinning as well. Therefore, the microstructure obtained by DCAP processes is more complicated and non homogeneous. In turn it shall result in more stabile and higher strength ultrafine-grained material structure.

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