# Evolution of perturbations of temperature and dislocation density at high-rate shear deformation of pure metals and alloys

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**Abstract** We have investigated numerically an evolution of initial perturbations of temperature or dislocation density in metals at high-rate deformation and its influence on the localization of plastic flow. A high-rate simple shear of micro-samples of pure metals and alloys, coarse-grained as well as nano-crystalline, has been simulated in two-dimensional geometry with use of the continuum mechanics supplemented by the dislocation plasticity and the grain-boundary sliding models. Perturbations of the temperature or dislocation density lead to restricted localization of the plastic deformation, but they can not initiate instability of the plastic flow as a self-sustained and increasing process. A more effective reason of the localization is the stress concentration, caused, for example, by boundary conditions. Rate of the plastic deformation is maximal in areas of the shear stress localization and it can be close to zero outside these areas. Heterogeneity of the grain sizes distribution through the sample can also lead to substantial localization of the plastic flow due to the grain size dependence of the dynamic yield strength.

Keywords High-rate plasticity, Localization, Temperature perturbation, Dislocations, Metals

# **1. Introduction**

Localization of macroscopic plastic deformation is a widespread phenomenon in metals. It can be provoked by decrease of the material temperature, by increase of deformation rate or by decrease of grain size in polycrystalline metals. Localization of the plastic flow manifests themselves as an appearance of local areas with high plastic deformation values - up to several tens. This phenomenon is being researched intensively [1-6]. Heterogeneities in form of narrow bands arising at the high rate deformation are known as adiabatic shear bands. They are two-dimensional and almost flat formations, which boundaries are displaced, one relative to another, like in cracks of the 2<sup>nd</sup> or 3<sup>rd</sup> type, but material between the boundaries remains continuous. Thickness of the bands usually varies from ten to several hundreds of micrometers, while an extent of the bands varies from several millimeters up to several centimeters. Up to 90% of the whole plastic deformation of the material can be concentrated in the shear bands, as well as high shear deformation is observed in the neighborhood of the bands [3]. Shear bands have a complex structure of highly deformed material and can contain dislocation arrangements and nanocrystalline grains inside themselves [7]. Such bands were observed in metallurgical processes for a long time and were described first by H. Tresca [8]. A hard striker breaking through the metallic barrier is another example of practically important process, in which localization is well defined and it was observed rather long ago [9,10]. Localization substantially effects on the material strength as a whole relative to shear deformation.

First important point in explanation of the shear bands formation was made by C. Zener and J.H. Hollomon [11], which had proposed that a local temperature rise during the deformation leads to softening of the material, and that competition between the temperature softening and a strain hardening results in instability of the plastic flow (thermoplastic instability) and in the localization [1,3]. This viewpoint had been supported by many authors and until recently it often was seen as only one possible. But in a large number of materials revealing the localization, the plastic deformation results in inessential temperature increase, which is not enough for a substantial

softening of a uniformly deformed material [12,13]. High-speed infrared photography have shown, that even in the areas of the plastic flow localization the temperature rise does not exceed 10 K in iron [14], while in titanium it is about 100 K [15]. Therefore, the thermoplastic instability could not be a universal mechanism of the localization.

At high-rate deformation of pure metals (at the strain rates about  $10^5$ - $10^6$  s<sup>-1</sup> or higher) a temperature hardening came in the stead of the temperature softening [16,17]. It is caused by an increase with temperature of friction force, which acts on moving dislocation [17,18]. Dislocations move in an over-barrier mode in the pure metals at such strain rates, and the dynamic yield stress is determined by the friction force and by the dislocation density. The transition to the over-barrier mode, revealing in the temperature hardening, can by expected in alloys as well but at the even more high strain rates. In conditions of the temperature hardening the thermoplastic instability scenario can not be truth. It also puts a question about place of the temperature perturbations and other factors in initiation of the localization.

Localization is often attended by a substantial change of defects substructure [7]. While the thermoplastic instability is theoretically well described, an influence of the defect substructure on the localization process is investigated on the level of estimations only. Objective of the present work was to investigate possible instabilities of plastic flow with respect to initial perturbations of temperature or dislocations density or the grain size in polycrystalline metals. We numerically studded a simple shear of pure monocrystalline aluminum, nanocrystalline aluminum and aluminum alloy. It is known that the pure aluminum is not inclined to the localization [19], while the aluminum alloys reveal it [20,21]. The obtained results, at first, seemed to be strange, but, in truth, fully explainable.

# 2. Model and formulation of problem

Total plastic deformation of the polycrystalline metals is supposed to be a result of the combined action of two competing effects, namely, the dislocation motion and the sliding along the grain boundaries. According to this viewpoint, the plastic deformation tensor  $w_{ik}$  is represented by the sum  $w_{ik} = w_{ik}^{D} + w_{ik}^{gb}$ , where  $w_{ik}^{D}$  is the part of plastic deformation caused by the dislocation motion, and  $w_{ik}^{gb}$  is the part caused by the grain boundary sliding. The dislocation plasticity [22,23] and the grain boundary sliding [24-26] models are generalized on the two-dimensional Cartesian case (2D) and used here for determination of  $w_{ik}^{D}$  and  $w_{ik}^{gb}$  correspondently. Full model consists of continuum mechanics equations supplemented by the equations for dynamics and kinetics of dislocations and by the equations for time derivatives of  $w_{ik}^{D}$  and  $w_{ik}^{gb}$ .

### 2.1. Equations system

Here we write down the equations system to be solved numerically below:

$$\frac{1}{\rho}\frac{d\rho}{dt} = -\frac{\partial v_k}{\partial x_k},\tag{1}$$

$$\rho \frac{dv_i}{dt} = \frac{\partial}{\partial x_k} \left( -P \cdot \delta_{ik} + S_{ik} \right), \qquad (2)$$

$$\rho \frac{dU}{dt} = \left(P + \frac{S_{ik}^2}{4G} + \varepsilon_D \rho_D\right) \frac{1}{\rho} \frac{d\rho}{dt} + \frac{\partial}{\partial x_l} \left(\kappa \frac{\partial T}{\partial x_l}\right) + S_{ik} \frac{dw_{ik}}{dt} - \varepsilon_D \frac{d\rho_D}{dt}, \qquad (3)$$

$$S_{ik} = 2G \left[ u_{ik} - \frac{1}{3} u_{ll} \cdot \delta_{ik} - w_{ik} \right], \tag{4}$$

$$\frac{du_{ik}}{dt} = \frac{1}{2} \left[ \frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} \right] + \Omega_{ik} , \qquad (5)$$

$$\frac{dw_{ik}^{\mathrm{D}}}{dt} = -\sum_{\beta} \frac{1}{2} \left( b_i^{\beta} n_k^{\beta} + b_k^{\beta} n_i^{\beta} \right) V_{\mathrm{D}}^{\beta} \rho_{\mathrm{D}}^{\beta} + \omega_{ik} , \qquad (6)$$

$$\frac{m_{0}}{\left[1 - \left(V_{\rm D}^{\beta} / c_{\rm t}\right)^{2}\right]^{3/2}} \frac{dV_{\rm D}^{\beta}}{dt} = \left(S_{ik}b_{i}^{\beta}n_{k}^{\beta} - \frac{bY}{2} \cdot \operatorname{sign}\left(S_{ik}b_{i}^{\beta}n_{k}^{\beta}\right)\right) - \frac{B \cdot V_{\rm D}^{\beta}}{\left[1 - \left(V_{\rm D}^{\beta} / c_{\rm t}\right)^{2}\right]^{3/2}},\tag{7}$$

$$\frac{d\rho_{\rm D}^{\beta}}{dt} = \frac{0.1}{\varepsilon_{\rm D}} \left\{ \frac{B \cdot \left(V_{\rm D}^{\beta}\right)^2}{\left[1 - \left(V_{\rm D}^{\beta} / c_{\rm t}\right)^2\right]^{3/2}} + b \cdot Y \cdot \left|V_{\rm D}^{\beta}\right| \right\} \cdot \rho_{\rm D}^{\beta} - k_a b \cdot \left|V_{\rm D}^{\beta}\right| \cdot \left(\rho_{\rm D}^{\beta}\right)^2, \tag{8}$$

$$\frac{dw_{ik}^{\rm gb}}{dt} = \frac{1}{2G\,\mathrm{T}} \sum_{\alpha} \tau_i^{\alpha} n_k^{\alpha} \left( S_{lm} \cdot \tau_l^{\alpha} n_m^{\alpha} - y_b \right) + \omega_{ik}^{\rm gb} \,. \tag{9}$$

where Eq. (1) is the continuity equation [27], Eq. (2) is the equation of motion, Eq. (3) is the energy conservation law, Eq. (4) is the generalized Hooke law [28] with accounting of the plastic strains  $w_{ik}$ , Eq. (5) is the equation for geometrical deformation  $u_{ik}$ , induced by a macroscopic motion of substance, Eq. (6) is the generalized Orowan equation [29] for the plastic strain  $w_{ik}^{D}$ , Eq. (7) and Eq. (8) are equations of dynamics and kinetics of dislocations [22]. Eq. (9) describes the grain boundary sliding [24-26], where T - relaxation time and  $y_{ik}$  - threshold stress for sliding.

In the Eq. (1) – Eq. (9):  $\rho$  is substance density;  $v_i = \{v_x, v_y, 0\}$  is velocity vector;  $x_i = \{x, y, 0\}$  are the Cartesian coordinates; P is the pressure, which is determined from a wide-range equation of state  $P = P(\rho, U)$  [30,31];  $S_{ik}$  is the tensor of stress deviators, which characterizes the shear stresses; U is the part of internal energy, which corresponds to the state with zero stress deviators  $S_{ik} = 0$  and with zero dislocation density  $\rho_D = 0$ ; T is the substance temperature, which also can be found from the wide-range equation of state  $T = T(\rho, U)$ ; G is the shear modulus;  $\kappa$  is the heat conductivity coefficient;  $\varepsilon_D \approx 8 \text{ eV}/b$  is the dislocation formation energy per unit length, where b is modulus of the Burgers vector of dislocation.

Tensors  $\Omega_{ik}$ ,  $\omega_{ik}^{\rm D}$  and  $\omega_{ik}^{\rm gb}$  take into account the change of  $u_{ik}$ ,  $w_{ik}^{\rm D}$  and  $w_{ik}^{\rm gb}$  correspondently due to substance rotation [32]. Indexes i, k, l, m numerate the space directions and run from 1 to 3; the summation rule is valid for dummy indexes;  $\delta_{ik}$  is the bivalent mixed tensor. Index  $\beta$ numerates possible slip systems of dislocations, which is characterized by the Burgers vector  $b_i^{\beta}$ and by the normal to the slip plane  $n_i^{\beta}$ . Dislocation density in the corresponding slip system is designated as  $\rho_{\rm D}^{\beta}$ , velocity of these dislocations -  $V_{\rm D}^{\beta}$ . Total density of dislocations can be obtained by summation  $\rho_{\rm D} = \sum_{\beta} \rho_{\rm D}^{\beta}$ . In the Eq. (7), Eq. (8):  $c_{\rm t} = \sqrt{G/\rho}$  is the transverse sound speed of the material;  $m_0 \approx 10^{-16}$  kg/m is the rest mass of the dislocations; Y is the static yield stress;  $k_a$  is the annihilation factor; B is the coefficient of phonon friction, it describes the resistance to the dislocation motion. Index  $\alpha$  numerates possible planes of grains sliding, which are characterized by the normal  $n_i^{\alpha}$ ;  $\tau_i^{\alpha}$  is the direction of maximal shear stresses in the  $\alpha$ -plane.

Eqs (1)-(8) were solved numerically with use of the computer program CRS, written by A.E. Mayer. Sub-problem of the substance dynamics (Eqs (1)-(3)) were solved by a modification of the numerical method proposed by A.P. Yalovets [33]. All other equations were solved by Euler method with a varied time step.

#### 2.2. Problem statement

Simple shear of 2D metallic sample with square cross-section is simulated (Fig. 1). One face of the sample ("lower" face, y = 0) is at rest v(y = 0) = 0, while the opposite face ("upper" face, y = L) moves along the "lower" face with constant velocity  $v_x(y = L) = L \cdot \mathcal{E}$  and  $v_y(y = L) = 0$ , where L is a lateral length of the square,  $\mathcal{E}$  is a shear deformation rate. The length L must be chosen small enough to provide disturbance propagation through the sample during a characteristic time of deformation (an inverse value to  $\mathcal{E}$ ), therefore, inequality  $L \leq 10^{-2} \cdot c_t / \mathcal{E}$  was required.

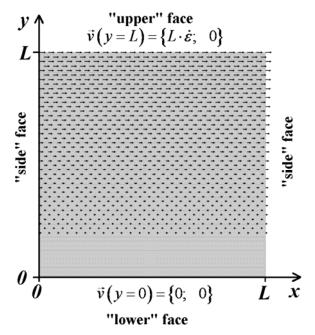


Figure 1. Initial state of the investigated 2D sample (initial velocity field is shown by little arrows).

Initial velocity was set linearly increasing from the "lower" face to the "upper" face:  $v_x(x, y) = y \cdot x v_y(x, y) = 0$ , which corresponds to a uniform simple shear, thus, an initial shear rate was uniform along the sample. Two different problems were determined by boundary conditions on the "side" faces: constrained shear – at the forced movement of the "side" faces with velocity  $v_x = y \cdot x v_y = 0$ ; and free shear – at free surface condition on it.

Pure aluminum, aluminum-copper alloy and ultra-fine-grained aluminum were studied. The pure aluminum was characterized by the next expression for the static yield stress  $Y_{Al} = 2.2 \cdot 10^7 + 0.4Gb \sqrt{\rho_D}$ . This expression takes into account the strain hardening (second term in the right-hand part) in a Taylor relation form [34]. The aluminum-copper alloy was characterized by

another expression for the static yield stress  $Y_{Al+Cu} = 28.625 \cdot 10^7 - 2.425 \cdot 10^5 \cdot T + 0.4Gb \sqrt{\rho_D}$ . First and second terms of the last expression represent a critical stress, which is necessary for dislocation detachment from inclusion. This critical stress depends on temperature; presented expression was obtained from molecular-dynamics simulations by A. Kuksin and A. Yanilkin [34]. The main differences between the pure aluminum and the aluminum-copper alloy in our study were the higher value of  $Y_{Al+Cu}$  in comparison with  $Y_{Al}$ , and the decrease of  $Y_{Al+Cu}$  with temperature. All other parameters (equation of state, friction coefficient of dislocation movement) were supposed to be the same for both materials. For the ultra-fine-grained and nanocrystalline aluminum the yield stress was chosen in the next form:  $Y_{Al} = 2.2 \cdot 10^7 + 0.4Gb \sqrt{\rho_D} + H / \sqrt{d}$ , where d is the grain size,  $H \approx 4.2$  GPa  $\cdot$  nm<sup>1/2</sup> is the Hall-Petch coefficient for aluminum.

Plastic strain intensity W was used as indicator of the state of plastic strain. In the 2D case it can be written as,  $W = \sqrt{(4/3) \cdot (w_{xx}^2 + w_{yy}^2 + w_{xx} \cdot w_{yy} + w_{xy}^2)}$ . Average value is determined as  $\langle W \rangle = A^{-1} \int_A W \cdot dA$ , where A is a cross-section of the sample (approximately  $A \approx L^2$  during the shear). Deviation of the plastic deformation from its average value is numerically characterized by the root-mean-square deviation  $\Delta W = \sqrt{A^{-1} \int_A (W - \langle W \rangle)^2 \cdot dA}$ .

The considered strain rate was equal to  $\&= 10^5 \text{ s}^{-1}$ , which value is typical for the high-speed impact experiments [17]. The sample size L was chosen equal to  $L = 100 \,\mu\text{m}$ ; the computational grid was 50x50 nodes. Initial perturbations were set in form of a narrow stripe (4  $\mu$ m width-way) parallel to Ox axis, which crosses the sample in its middle. In this stripe, either the initial temperature of substance was raised on  $\Delta T$ , or the initial dislocation density was multiplied on factor  $(1 + \Delta \rho_D / \rho_D)$ , where  $\rho_D$  is an unperturbed value of the dislocation density,  $\Delta \rho_D$  is its perturbation; the value  $\rho_D = 10^7 \,\text{cm}^{-2}$  was used in calculations below. In nanocrystalline aluminum perturbation of the grain size was also investigated – grain size inside the stripe was set equal to  $d_1$ , which value is different from the grain size outside the stripe d.

## 3. Results and discussion

It was supposed, that if the specified perturbation is appropriate and enough for localization of plastic flow, then the upper half of the sample will plastically displace relative to the lower half at the free shear. But numerical experiments have shown that the initial perturbations of temperature or dislocation density influence on the localization of plastic flow only at the constrained shear mode. Therefore, we will consider results of the constrained shear at first.

Fig. 2 shows typical distributions of the plastic strain intensity for alloy and pure aluminum with initially perturbed temperature field. Raise of temperature in the alloy leads to decrease of the yield stress, and plastic deformation tends to be localized in the hot stripe (Fig. 2(a)). Constrained movement of the "side" faces suppresses total plastic shear along this stripe, therefore, the plastic deformation redistributes around the stripe, which, particularly, cause formation of arrowhead-like structures. Plastic deformation in vicinity of the hot stripe (aside from the arrowhead-like areas) is lower then the plastic deformation near the "upper" and "lower" faces. An inverse situation takes place for the pure aluminum (Fig. 2(b)). Rise of temperature increases the resistance to dislocations

motion and suppresses the plastic deformation inside of the hot stripe. For compensation of this effect, a more intensive plastic flow occurs in its vicinity. It can be treated as localization as well, not in the hot stripe, but around the stripe (around the perturbed area).

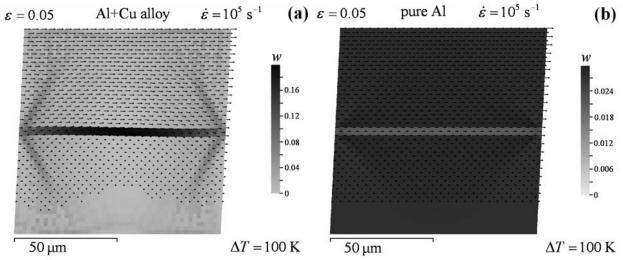


Figure 2. Distributions of the plastic strain intensity w in the aluminum-copper alloy (a) and in the pure aluminum (b) samples at the total deformation  $\varepsilon = 0.05$ . Initial temperature field was perturbed by narrow (4 µm) stripe with temperature raised on  $\Delta T = 100$  K; constrained shear.

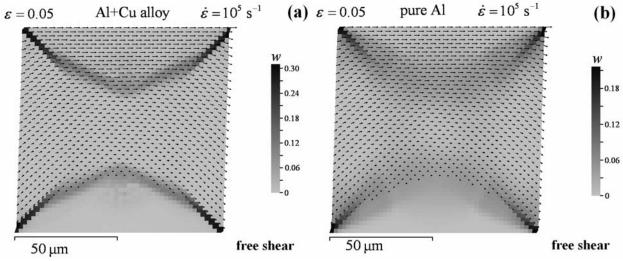


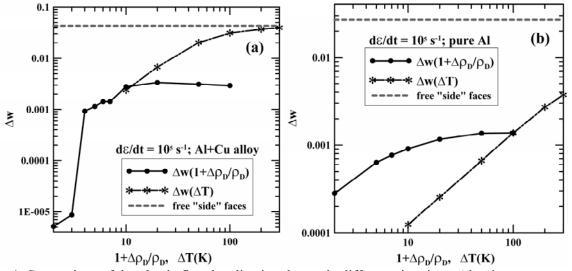
Figure 3. Distribution of the plastic strain intensity w in the aluminum-copper alloy (a) and in the pure aluminum (b) at the free shear are presented at the shear deformation  $\varepsilon = 0.05$ . Both in alloy and in the pure metal, localization begins along diagonals of the square.

Calculations show that substantial localization takes place only at  $\Delta T$  above several tens or hundreds of K, while the plastic flow causes an increase of temperature on only about several K. These facts indicate that any random disturbance in temperature can not of itself lead to a self-sustained process of the connected temperature rise and temperature softening of the material. In other words, temperature perturbation can not initiate instability of plastic flow even in alloys. But pre-existing areas with substantially different temperature can in some degree localize the plastic flow around themselves both in alloys and in pure metals. The degree of localization in the pure metal is on an order of magnitude less than that in the alloy.

Increase of the initial dislocation density leads to a temporary softening of pure metal at dynamic

deformation, therefore, plastic deformation is higher in the perturbed stripe with the higher initial dislocation density and it is lower in the attached areas. This is a temporary effect, and it becomes lower with the increase of total deformation. It is explained by the fact that the dislocation density grows up, and the softening (a dynamical effect) is replaced by an increase of the yield stress with dislocation density (a strain hardening). In the case of alloy, the higher value of the yield strength causes an earlier transition to the strain hardening. As opposed to the temperature, the dislocation density changes substantially during the plastic flow. But it seems that the plastic flow instability can not be provoked by the dislocation density perturbation as well as in the temperature perturbation case. At the dislocation-induced softening the dislocation density growth diminishes the softening effect. At the strain hardening the "inverse" localization takes place, but more intensive plastic deformation around the perturbed area increases the dislocation density in this surroundings. It leads to an equalizing of the dislocation density and to a broadening of the involved area, it means, to delocalization. Meanwhile, an irregularity in the dislocations distribution leads to some localization of the plastic deformation, but this localization is restricted.

Much more localization takes place at the free shear (Fig. 3). Both in alloy and in the pure metal, localization begins along diagonals of the square. Region at rest near the "lower" face, region moving with constant velocity & L near the "upper" face and a flowing central region appear as a result of development and intersection of the localization bands. In the alloy localization is stronger than in the pure metal. It must be emphasized, that the localization at free shear arises without any initial perturbation of the initial parameters. Moreover, any perturbation of temperature or dislocation density does not effect in this case.



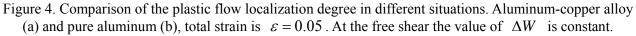


Fig. 4 presents a comparison of the plastic flow localization degree produced by various initial perturbations of dislocation density or temperature at the constrained shear and the localization at the free shear. In the alloy, the temperature perturbations with  $\Delta T > 10$  K are substantially more effective than the dislocation density perturbation (Fig. 4(a)). At the temperature increase on  $\Delta T \approx 300$  K the degree of localization tents from bellow to the localization degree at the free shear. But it seems hardly probable that such high temperature drop can initially exist in the material. In the pure aluminum, the dislocation density perturbation is more effective from the viewpoint of the localization excitation than the temperature increase with  $\Delta T < 100$  K (Fig. 4(b)); but the free shear is much more effective than the both types of perturbations.

Perturbation of the grain size in ultra-fine-grained or nano-crystalline aluminum leads to substantial localization of the plastic flow at the "constrained" shear due to difference in the dynamical yield strength. Localization degree in nano-materials with the grain size d < 100 nm depends weakly on the perturbation value  $d_1/d$ , therefore, localization in such materials has to arise at any arbitrary size distribution of the grains. But the localization degree is all the same less than it at the "free" shear; they become comparable only at the grain size d < 10 nm.

## 4. Conclusions

Summarizing, one can conclude that perturbation of both the temperature and the dislocation distribution, as well as of the grain size, can lead to restricted localization of the plastic flow. But they can not initiate the self-sustained process of the joint increase of corresponding parameter and of the localization degree, it means, they can not initiate the instability of plastic flow. Nonuniformity of acting stresses is the dominant factor of the localization of the plastic deformation. Therefore, the process of localization must substantially depend on the loading conditions and on the internal structure of the material (on the presence of inhomogeneities, pores, inclusions).

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