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The dynamics of dislocation wall generation in metals and alloys under shock loading

E.A. Rzhavtsev[a] and M.Yu. Gutkin[a,b,c,*]

[a]*Department of Mechanics and Control Processes, St. Petersburg Polytechnic University, Polytekhnicheskaya 29, St. Petersburg 195251, Russia*
[b]*Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vasil. Ostrov, St. Petersburg 199178, Russia*
[c]*ITMO University, Kronverkskiy pr. 49, St. Petersburg 197101, Russia*

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Two-dimensional discrete dislocation–disclination dynamics is applied to model the formation of dislocation walls in shock loaded metals and alloys. The dislocation walls are generated under an external stress impulse and the stress fields of pre-existed wedge disclinations distributed over the subgrain boundary. The case of an aluminum alloy is analyzed. It is shown that the typical shock duration is enough to complete the fragmentation process within the initial subgrain, and the necessary stress magnitude well agrees with experiments.

Keywords: Alloys; Dislocation boundaries; Dislocation dynamics; Disclinations; Shock loading

The study of microstructural changes in metals and alloys during plastic deformation is one of fundamental problems in the physics of strength and plasticity. In recent years, much attention has been attracted to the severe plastic deformation processes of obtaining ultrafine-grained and nanostructured materials as they have a number of useful mechanical properties and prominent applications (see, for example, reviews [1–6] and a recent book [7]). These processes commonly include the stage of dynamic recrystallization which is therefore of great interest today [8]. In particular, the phenomenon of dynamic recrystallization in shear bands which appear in metals and alloys under shock loading, has been in the focus of extended research.

Some of the earliest observations of dynamic recrystallization in shear bands formed in Ti–6Al–4V and commercial purity titanium under shock compression, were made by Grebe et al. [9] and by Meyers and Pak [10,11], respectively. Identical processes in shock-conditioned copper and tantalum were first observed by Andrade et al. [12] and by Nesterenko et al. [13], respectively. Recently Meshcheryakov et al. [14,15] reported that under certain conditions of shock compression, the dynamic recrystallization was also observed in the shear bands in the D16 aluminum alloy.

A theoretical model of dynamic recrystallization in shear bands under shock compression was suggested long before by Grebe et al. [9]. These authors subdivided the recrystallization process into five main stages of which the grain fragmentation (grain division into misoriented fragments) was considered as a key intermediate stage. However, the fragmentation process itself was not described in detail in this model. Moreover, in spite of long-term investigations of fragmentation, started in the mid of 1970-s [16–19], its theoretical description is still quite far from total clarity. A great progress in its understanding was achieved after introduction of the concept of partial disclinations which are treated as the principal carriers of plastic deformation in metallic materials at the fragmentation stage [20–24]. In recent years, an effective tool in theoretical modeling of partial disclinations and fragmentation development has become the approach of 2D discrete dislocation–disclination dynamics (the D^4-approach) which describes the collective behavior of straight dislocations interacting with partial disclinations and, moreover, forming these disclinations [23,25–32]. This approach is a natural extension of the well-known 2D discrete dislocation dynamics [33–38] (see also [39] for more references) to the case of large plastic deformations. It is also worth noting that until now, the 2D D^4-approach has been applied to simulations in quasi-static conditions under which the fragmentation process develops during hundreds of seconds [28–32]. In the shock-loading experiments of interest [14,15], the duration of the impact impulse was of about 650 ns and, therefore,

* Corresponding author at: Department of Mechanics and Control Processes, St. Petersburg Polytechnic University, Polytekhnicheskaya 29, St. Petersburg 195251, Russia.; e-mail addresses: egor.rzhavtsev@gmail.com; m.y.gutkin@gmail.com

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the fragmentation stage of observed dynamic recrystallization had to be even shorter.

The aim of the present work is to simulate the fragmentation process within pre-existing subgrains in shear bands in metallic materials under shock loading by means of the 2D D^4-approach. We suggest a computer model, clearly demonstrating the fragmentation process through the formation and evolution of the walls and arrays of edge dislocations under the action of an external stress impulse and the stress fields of various configurations of pre-existing wedge grain-boundary disclinations generated during the pre-existing subgrain formation. Our modeling shows that (i) the shock duration used in experiments [14,15] is enough to complete the fragmentation process within the initial subgrain, and (ii) the necessary stress impulse magnitude well agrees with that which was used in these experiments.

The main idea of the model is illustrated by Figure 1 which images a pre-existing elongated subgrain which has been formed at the first stage of model [9] under highly non-equilibrium conditions of shock wave propagation and, therefore, can contain many jumps of misorientation angles $\theta_1, \ldots, \theta_7$ at the subgrain boundaries formed by chaotically stored dislocations. In the case of tilt boundaries, the jump points are effectively described in terms of partial wedge grain-boundary disclinations [20,21] which are marked by black and white triangles in Figure 1 and are characterized by strengths $-\omega_1 = \theta_2 - \theta_1$, $\omega_2 = \theta_3 - \theta_4$, etc. These disclinations can capture the dislocations gliding nearby within the subgrain and make them to form new dislocation walls which are, in fact, fragment boundaries. A similar but periodic initial disclination structure with an equal magnitude ω of the disclination strengths was used in quasi-static computer simulations [31]. This process represents the physical mechanism of grain fragmentation at the second stage of dynamic recrystallization in model [9].

Our simulation was performed for different self-screened configurations of the initial disclination structures [21], in which case the total strength of the disclinations is zero. Firstly, we considered a biaxial disclination dipole with the arm d and disclination strengths $\pm\omega$ (Fig. 2a). In the rectangular simulation box imaging the initial subgrain, the positive disclination lies on the z-axis of the Cartesian coordinate system, while the negative one passes through the point $(x = 0,\ y = d)$. Far from the dipole, on the lines $(x = \mp x_0,\ 0 < y < d)$, at the time $t = 0$ under an applied shear stress τ starts generation of "positive" and "negative" edge dislocations with Burgers vectors $\pm\mathbf{b}$ directed along the x-axis, respectively. The initial distribution of dislocations along the y-axis and the moments of their appearance are given by the random number generator. The planes $y = \text{const}$ are the slip planes for the dislocations. It is assumed that dislocations of opposite signs are annihilated when the distance between them becomes less than $3a$, where a is the lattice parameter.

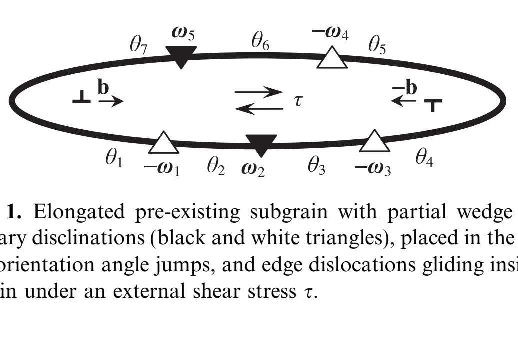

Figure 1. Elongated pre-existing subgrain with partial wedge grain-boundary disclinations (black and white triangles), placed in the points of misorientation angle jumps, and edge dislocations gliding inside the subgrain under an external shear stress τ.

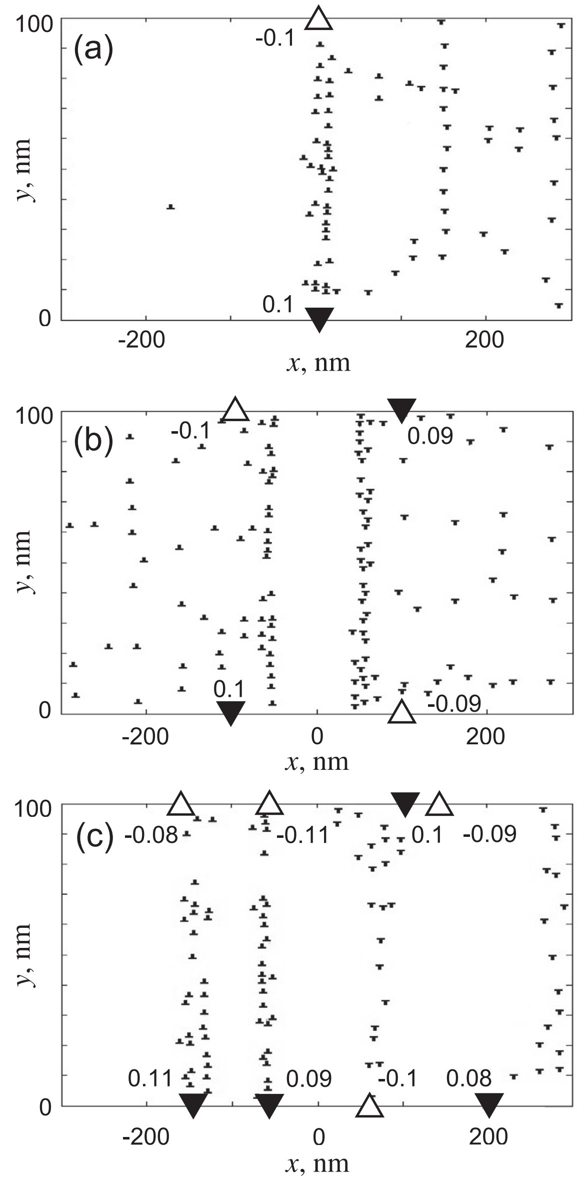

Figure 2. Stable dislocation structures formed after 10 ns under the applied shear stress 0.5 GPa in the stress fields of (a) a dipole, (b) a quadrupole, and (c) a random octupole of partial wedge disclinations. The disclination strengths are shown in radians at the disclination symbols (black and white triangles).

Each dislocation in the presented model is under the action of forces caused by the applied shear stress τ and stress fields of other dislocations and disclinations. Within the assumption that the dislocations slip only in planes $y = \text{const}$, their motion is determined by the x-components of these forces. The motion equation for the i-th dislocation then reads [26]:

$$m\frac{d^2x_i}{dt^2} + \beta\frac{dx_i}{dt} = F_i, \quad i = 1, 2, \ldots N, \tag{1}$$

where m is the effective mass of the dislocation, x_i is its coordinate, β is the dynamic friction (drag) coefficient, F_i is the total force on the dislocation, and N is the number of dislocations generated during one experiment. The dislocation mass is $m = \rho b^2/2$ [40], where ρ is the material density.