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The study on the effect of the dislocation density on formation of a closed piecewise-continuous dislocation loop in aluminum

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Abstract. Mathematical model allowing carrying out studies on energy, scale and time characteristics of formation of closed dislocation loop and crystallographic shear zone as a whole, and forming of a dislocation loop for FCC-materials, has been developed. Using the mathematical model study on the effect of the dislocation density on the dynamics of formation of an elementary crystallographic slip bounded by a closed piecewise-continuous dislocation loop in aluminum has been carried out. It has been shown that with decrease in the density of dislocations in metal from 10^{-12} up to $4 \cdot 10^{-11}$ along different orientations of the expansion of the dislocation loop the maximum value of the dislocation velocity increases by 20-30% and the maximum value of the kinetic energy and the dislocation path increases by almost 2 times. It has been shown that in aluminum the area of elementary crystallographic slip, swept out by the dislocation loop, increases with a decrease in the dislocation density in metal. But, at the same time, regardless of the value of the dislocation density in metal the radius of the dislocation loop in the final configuration along the screw orientation is practically by an order of magnitude less than along the edge orientation.

1. Introduction

Studies on strength and plasticity of metals on the basis of the dislocation theory have a long history. The number of proposed dislocation mechanisms, experimental observations, and theoretical calculations is very large. But in view of the complexity of studies on the dynamics of dislocations this line of research is still relevant.

Peculiarities of formation of a dislocation structure depend on various factors, including: the applied stress, the temperature, and the dislocation density in material, as well as many others. During the expansion the dislocation loop overcomes many obstacles of various nature and strength [1–3]. For several reasons the dislocation is usually not the only one. A series of dislocations that form the crystallographic shear zone occurs at a high velocity (significantly higher than the velocity of the macroscopic strain) as a result of the stability loss by a dislocation source. In turn, stress fields that occur during formation of the crystallographic shear zone can activate other dislocation sources, resulting in expansion of plastic strain autowaves along the strained crystal [4]. The dynamic behavior of the dislocation under conditions of the stability loss can lead to multiple effects that cannot be predicted within the framework of the conventional concept of the stationary thermally activated motion of dislocations [5, 6].

2. Mathematical model of the dislocation dynamics

To describe the dynamics of expansion of dislocation loops emitted by one dislocation source and formation of the crystallographic shear zone a mathematical model has been developed [7], which enables to study energy, scale and time characteristics of a closed piecewise-continuous dislocation loop in FCC-metals:

$$d\varepsilon_k^{(j)}\big/dt = \left[\frac{1}{4}(\pm\tau b - \tau_R b - Bv^{(j)})T^{(j)} - \left(8\sigma\sqrt{2\pi}\right)^{-1} e^{-\frac{\sin(\beta^{(j)})^2}{2\sigma^2}} p_j p_s \xi Gb^2\rho r^{(j)} \mp \right.$$

$$\left. \mp \frac{Gb(i-1)\left(\cos^2(\beta^{(j)}) + \sin^2(\beta^{(j)})/(1-\nu)\right)}{2\pi(r_1^{(j)} - r^{(j)})} \mp \frac{(\mu_0^{(j)} + \varepsilon_k^{(j)})}{2}Q^{(j)}\right]v^{(j)}, \; j = \overline{1,m} \qquad (1)$$

$$dr^{(j)}\big/dt = \pm v^{(j)}, \; j = \overline{1,m}.$$

where $r^{(j)}, v^{(j)}, \varepsilon_k^{(j)}$ are: the current radius, the velocity, and the kinetic energy along the *j*-th orientation; *t* is the motion time of the dislocation loop; τ is the applied stress; τ_R is the stress of the lattice strain and the impurity strain, and the dislocation resistance to the dislocation motion; *G* is the shear modulus; *b* is the Burgers vector module; *B* is the coefficient of the viscous deceleration of the dislocation; ρ is the density of dislocations in the material; p_j is a fraction of jog-forming dislocations of non-coplanar systems, p_s is a fraction of jogs located on near-screw segments of the dislocation loop, ξ is the Smallmen factor; ν is the Poisson's ratio; σ is the dispersion of a normal distribution of the intensity of point defect generation beyond jogs on the dislocation; $T^{(j)}$, $Q^{(j)}$ is the combination of physically determined parameters [7]; $\mu_0^{(j)}$ is the linear tension of the stationary immobile dislocation; $\beta^{(j)}$ is the angle between the Burgers vector and the normal to the *j*-th orientation; $\beta^{(m+1)} = \beta^{(1)}$; $r^{(m+1)} = r^{(1)}$, *m* is the number of sides of the polygonal shape of the dislocation loop.

When writing the mathematical model (1) an assumption was used that the calculation was carried out in a polar coordinate system, and the dislocation loop in the initial configuration was represented in the form of a regular polygon with infinitely small sides and the center coinciding with the center of the coordinate system. For the dislocation loop, the boundary components are normal to the polar axis, the screw components are parallel to it, and the generation of point defects, according to the experimental data [8], is carried out mainly within the limits of 15° from the screw orientation of the dislocation loop.

In the model (1) Peach-Koehler forces are taken into account, as well as the dissipative forces caused by: the lattice, the impurity and dislocation deceleration; the linear tension; the viscous deceleration; the stress from accumulation of dislocations and generation of point defects beyond jogs on the dislocation. Besides, the dependence of the linear tension and the intensity of generation of point defects on the orientation of the Burgers vector with respect to the dislocation line are taken into account.

The article presents the results of the study on the evolution of the first dislocation loop emitted by a dislocation source at various densities of dislocations in aluminum, obtained using the mathematical model (1).

3. Results of the computational experiment

For implementation of the mathematical model (1) and implementation of computational experiments a set of software (Dislocation Dynamics of Crystallographic Slip [9, 10]) has been created, which implements the most appropriate for the solution of the system (1) numerical Gere method of the variable order and the integration step. The software complex has a developed user interface that allows researchers without a broad experience in programming and knowledge in the field of numerical methods to work with a set of programs.

Computational experiments have been carried out at values of parameters of the mathematical model specific to aluminum at room temperature: the stress of the lattice and impurity deceleration of

1 MPa acting on the dislocation source with a stress of 10.7 MPa (equal to the critical stress of a dislocation source at a dislocation density of 10^{12} m^{-2}). The density of dislocations in metal in various calculations has ranged from $4 \cdot 10^{11}$ m^{-2} up to 10^{12} m^{-2}.

As the result of the carried out study it has been shown that the dislocation loop, emitted by a dislocation source, quickly gains the terminal velocity (Figure 1, *a, d*), which is consistent with the experimental results [11]. At the same time, the terminal velocity of the dislocation is nearly by an order of magnitude less than the transverse sound velocity in metal.
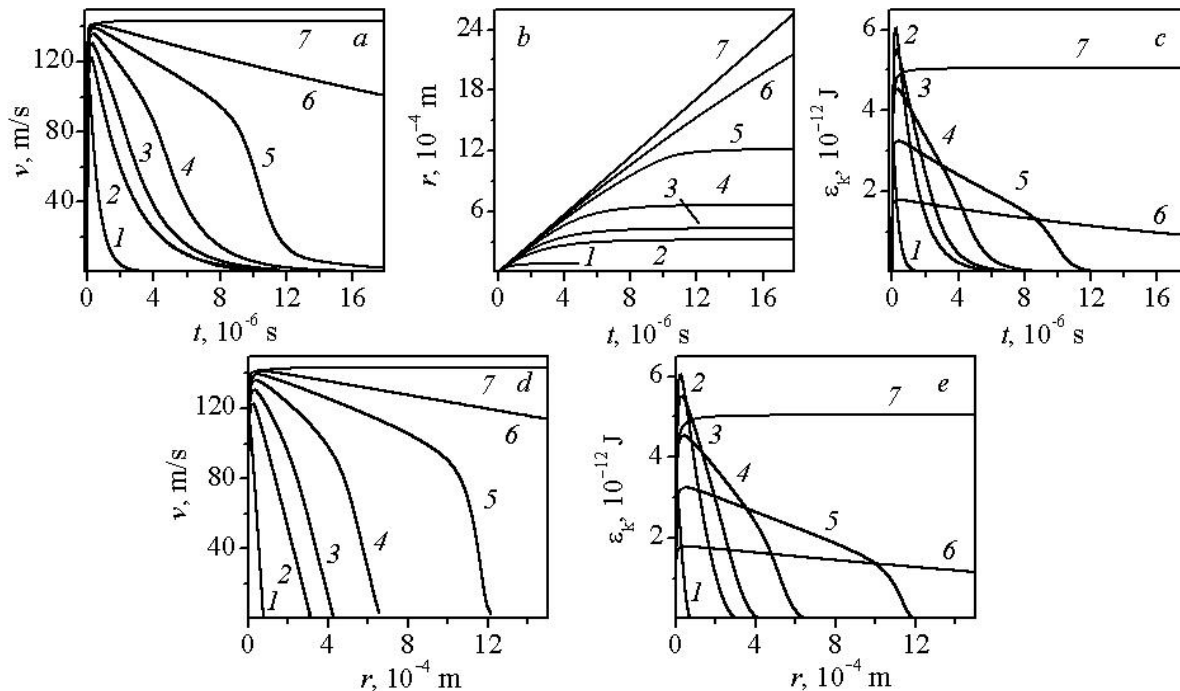
Figure 1. The dependency of the current velocity (*a*), the dislocation radius (*b*), and the kinetic energy (*c*) per unit length of the dislocation on the path time, and the dependency of the velocity (*d*) and the kinetic energy (*e*) per unit length of the dislocation on the dislocation radius in aluminum along different orientations of the dislocation loop: *2* – β = 0° (screw dislocation), *3* – β = 30°, *4* – β = 45°, *5* – β = 60°, *6* – β = 90° (edge dislocation).

The velocity of the dislocation loop decreases after reaching the limiting value at the initial path of the dislocation. A three-stage decrease in the velocity is clearly observed in the dislocation along the edge and nearby orientations: 1) the stage of slow decrease in the velocity; 2) the stage of rapid decrease in the velocity; 3) the stage of the dislocation deceleration. The closer the orientation of the dislocation loop to the orientation of the edge dislocation, the slower the velocity decreases at the stage 1, the faster the velocity decreases at the stage 2, and, hence, the stage 3 is shorter. The velocity of the dislocation along the screw and nearby orientations after reaching the terminal velocity at the initial path significantly decreases, reaching a value close to zero, and a long-term stop of the dislocation takes pace (Figure 1, *a, d*).

The radius of the dislocation increases quasi-linearly along the edge and nearby orientations of the dislocation loop. For dislocations along other orientations, after the stage of an increase in the radius, a deceleration stage is observed at which the radius remains practically unchanged (Figure 1, *b*). At the same time, the deceleration stage becomes more pronounced at a decrease in the angle between the dislocation line and the Burgers vector (angle β).

At the initial path of the dislocation loop a sharp increase in the kinetic energy per unit of the dislocation length along all orientations is observed, alternating with a smooth decrease in the kinetic energy. The smaller the angle between the dislocation line and the Burgers vector, the greater the

maximum value of the kinetic energy; and for the screw dislocation it is almost 3 times greater than for the edge dislocation. Further expansion of the dislocation loop leads to a decrease in the kinetic energy along all orientations; and the greater the limiting value of the kinetic energy of the dislocation, the higher the rate of a decrease in the kinetic energy (Figure 1, *c*, *e*).

As a result of the carried out study it has been shown that the velocity and the radius of the dislocation, as well as the kinetic energy per unit length of the dislocation, increase along all orientations at a decrease in the density of dislocations in metal at the same path time and path length, (Figure 2).
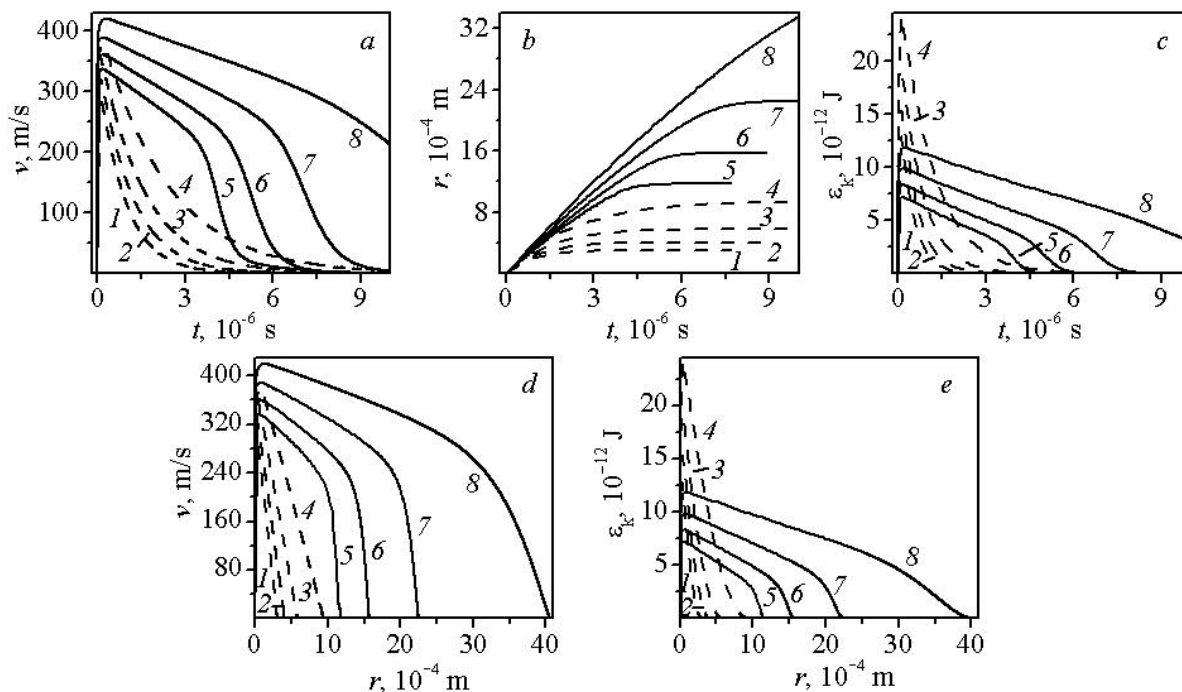

Figure 2. The dependency of the current velocity (*a*), the radius of the dislocation (*b*), and the kinetic energy (*c*) per unit length of the dislocation on the path time, and the dependency of the dislocation velocity (*d*) and the kinetic energy (*e*) per unit length of the dislocation on the dislocation radius in aluminum at various densities of dislocations in metal m^{-2}: $1, 5 - 10^{-12}$, $2, 6 - 8 \cdot 10^{-11}$, $3, 7 - 6 \cdot 10^{-11}$, $4, 8 - 4 \cdot 10^{-11}$; and along various orientations of the dislocation loop: broken curve − β = 0° (screw dislocation), continuous curve − β = 60.

For the screw dislocation, with a decrease in the density of dislocations in metal from 10^{-12} up to $4 \cdot 10^{-11}$ the maximum value of the velocity increases by nearly 30%, the kinetic energy – practically by 2 times, and the radius increases by more than 2 times. For the edge and mixed dislocations, with a decrease in the density of dislocations in metal from 10^{-12} up to $4 \cdot 10^{-11}$ the maximum value of the velocity, the kinetic energy, and the path length of the dislocation is slightly smaller (the difference is 15 % maximum) than for the screw dislocation. At a decrease in the dislocation density a three-stage decrease in the velocity of mixed dislocations, observed after reaching a limiting value of the velocity at the initial path of the dislocation, becomes less pronounced (Figure 2, *a*), the velocity and the kinetic energy decrease, and the radius increases more evenly (Figure 2, *b–e*) .

It has been shown that at the initial path the dislocation loop has the shape close to elliptical with a minor semi-axis perpendicular to the Burgers vector (Figure 3, *a*). After the initial path along the screw and nearby orientations in aluminum as well as in copper [7] a concavity area in the dislocation loop occurs (Figure 3, *b*), increasing until the dislocation stops (Figure 3, *c*, *d*). In the final configuration, the radius of the dislocation loop along the screw orientation is practically by an order

of magnitude less than along the edge orientation. The width of the dislocation loop increases along all orientations at a decrease in the dislocation density in material and at the same path time.
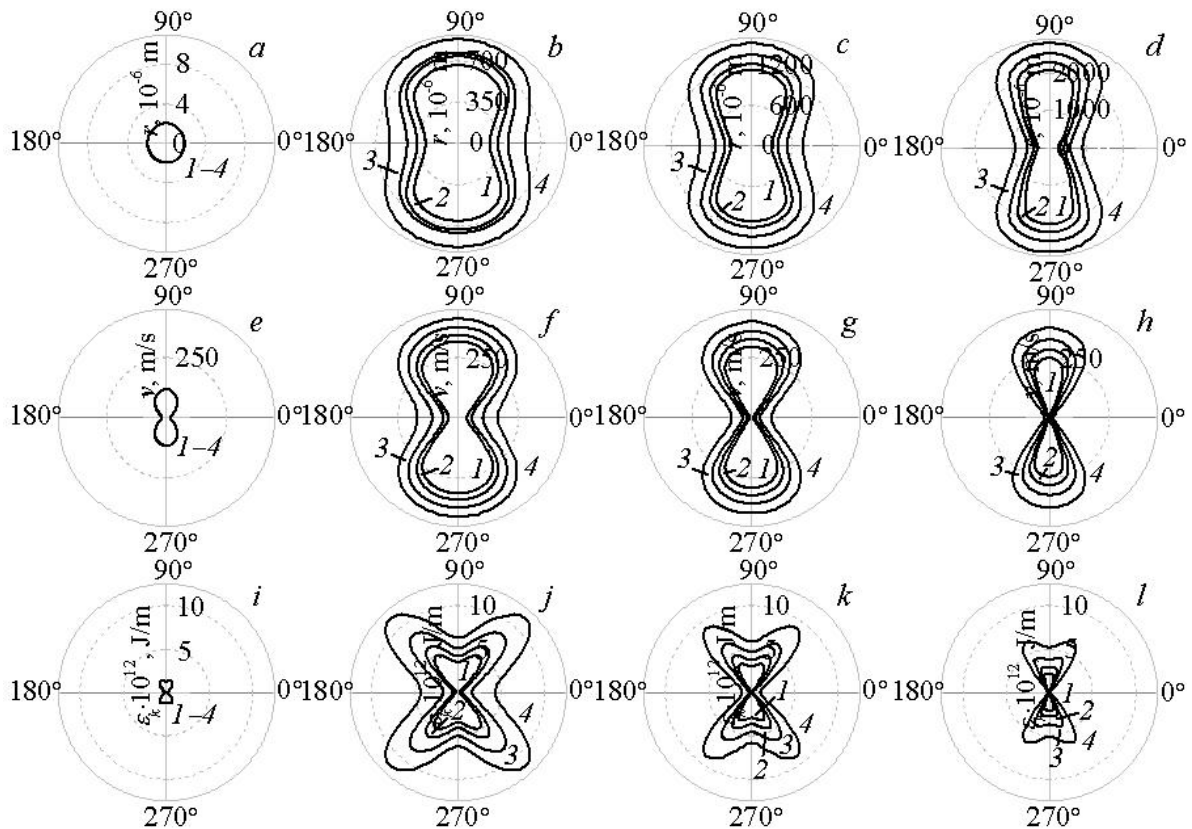
Figure 3. The shape of the dislocation loop, the velocity, and the kinetic energy per unit length of the dislocation loop along various orientations in aluminum, calculated at different time points from the beginning of the motion, s: $a, e, i - 10^{-9}$; $b, f, j - 2 \cdot 10^{-6}$; $c, g, k - 3.5 \cdot 10^{-6}$; $d, h, l - 7 \cdot 10^{-6}$; at various density of dislocations, m^{-2}: $1 - 10^{-12}$, $2 - 8 \cdot 10^{-11}$, $3 - 6 \cdot 10^{-11}$, $4 - 4 \cdot 10^{-11}$.

The expansion velocity of the dislocation loop is maximal in the direction of the edge and nearby orientations, and is minimal in the direction of the screw orientation (Fig. 3, *e–h*). Deceleration of the dislocation loop along the screw orientation is caused by the intensity of generation of point defects beyond jogs on the dislocation. The edge dislocation is stopped by the action of the linear tension during deceleration of the dislocation loop along other orientations. Both of these factors affect mixed dislocations in a proportion that depends on the proximity to the screw or the edge orientation. The kinetic energy per unit length of the dislocation loop, on a larger part of the path, has a maximum value in the direction of 60–70° from the screw orientation of the dislocation (Figure 3, *i–l*), reaching the value 1.5–2 times higher than the kinetic energy along the edge orientation (Figure 3, *j*). During deceleration of the dislocation loop the kinetic energy per unit length of the dislocation decreases the quickest along the screw and nearby orientations (Figure 3, *k, l*). With a decrease in the density of dislocations in aluminum the velocity and the kinetic energy of the dislocation loop increases along all orientations.

4. Conclusion

As a result of the carried out study it has been shown that a decrease in the density of dislocations in metal leads to an increase in the velocity and the radius of the dislocation, as well as the kinetic energy per unit length of the dislocation. With a decrease in the dislocation density in metal from 10^{-12} m^{-2} up to $4\cdot10^{-11}$ m^{-2} along different orientations of expansion of the dislocation loop the maximum velocity of the dislocation increases by 20–30% , the maximum value of the kinetic energy and the dislocation path increase by almost 2 times. It has been shown that in aluminum, as well as in copper, at the initial path the shape of the dislocation loop, initially presented in the form of a regular polygon, is close to elliptical with a minor semi-axis perpendicular to the Burgers vector. After the initial path a concavity area of the dislocation loop occurs, increasing until the dislocation stops. The area of the elementary crystallographic slip, swept out by the dislocation loop, increases with a decrease in the density of dislocations in metal. The radius of the dislocation loop in the final configuration along the screw orientation is almost by an order of magnitude less than along the edge orientation, regardless of the value of the dislocation density.

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