The Dynamics of Near-Surface Prismatic Loops in Lead

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Abstract. The paper proposes the study of the dynamics of near-surface dislocation loops in lead. It has been shown that the activation of a prismatic near-surface dislocation loop and its motion inward the crystal practically throughout the entire path occurs at a high velocity close to the speed of sound in metal. The kinetic energy per unit length of the dislocation loop during its motion decreases linearly and weakly depends on the density of dislocations in metal. Moreover, a weak dependence of the path length and the path time of a prismatic loop on the dislocation density in lead is observed.

INTRODUCTION

One of the most common phenomena of a plastic form change of crystalline solids is a crystallographic slip [1–4]. However, under different conditions a significant contribution to the dynamics of dislocations is made by other mechanisms [5]. Thus, the mechanical impact on a crystal leads to formation on its surfaces of closed prismatic dislocations with the Burgers vector perpendicular to the bedding plane of the loop. A prismatic dislocation loop during its occurrence is often under high stress. The source of an increased local stress can be the vertex of the cone, the indenter pyramid or the micro-roughness of the sample. The appearance of prismatic loops on the surface of a crystal is one of the mechanisms of change in the relief. The given deformation mechanism contributes to accommodative processes taking place at all the mechanical interactions: collision of two crystalline solids, deformation of small particles, metal treatment under pressure, etc. [6].

MATHEMATICAL MODEL

The dynamic equation of a dislocation prismatic loop formed near the surface of a crystal is presented in the form [6]:

$$\frac{d\varepsilon_k}{dz} = -\tau_R b - B\upsilon ,$$

where ε_k is the kinetic energy per unit length of the dislocation, z is the coordinate of the center of the dislocation loop, $\tau_R = \tau_f + \alpha G b \rho^{1/2}$ (τ_f is the friction stress, G is the shear modulus, b is the modulus of the Burgers vector, ρ is the density of dislocations, α is the parameter of the intensity of interactions among dislocations), B is the viscous friction coefficient, υ is the dislocation velocity.

For a full energy of the moving dislocation we shall use a pseudo-relativistic ratio $\varepsilon = \varepsilon_0 (1-\upsilon^2/c^2)^{-1/2}$, where c is the speed of sound in metal [7]. Thus, we obtain:

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$$\frac{d\varepsilon_k}{dz} = -\tau_R b - Bc\sqrt{1-\left(1+\frac{\varepsilon_k}{\varepsilon_0}\right)^{-2}} \tag{1}$$

To obtain a dependence of the kinetic energy and the dislocation path on the time, using the correlation $dz = \upsilon dt$, we shall represent the equation (1) as an equivalent system of equations:

$$\begin{cases} \dfrac{d\varepsilon_k}{dt} = \left(-\tau_R b - Bc\sqrt{1-\left(1+\dfrac{\varepsilon_k}{\varepsilon_0}\right)^{-2}}\right)\cdot\left(c\sqrt{1-\left(1+\dfrac{\varepsilon_k}{\varepsilon_0}\right)^{-2}}\right), \\ \dfrac{dz}{dt} = c\cdot\sqrt{1-\left(1+\dfrac{\varepsilon_k}{\varepsilon_0}\right)^{-2}}. \end{cases} \tag{2}$$

The dislocation loop formed at a stress concentrator near the surface of the crystal accelerates in the vicinity of the concentrator at stresses reaching the values close to the theoretical limit of the crystal strength. Dislocations acquire a high kinetic energy in the field of the concentrator, which allows them to penetrate far into the volume of the crystal. When moving from the surface depthward the crystal the dislocation works against forces conditioned to the lattice friction, elastic fields of impurity atoms, dislocations of non-complanar slip systems, the scattering of phonons and conduction electrons.

The magnitude of the kinetic energy per unit length of the prismatic loop, formed as a result of the shear stability loss by the crystal lattice, is determined by forces acting on this section in the field of the stress concentrator, i.e.,

$$\varepsilon_k^{(0)} = b\left|\int_0^\delta \tau_c(z)dz\right|,$$

where τ_c is the stress near the concentrator, δ is the "size" of the stress concentrator. The field of the stress concentrator fades at distances of an order of the characteristic scale of the concentrator. Taking this into account, we shall estimate the value of the kinetic energy per unit length of a heterogeneously originated dislocation as follows:

$$\varepsilon_k^{(0)} \approx \frac{Gb\delta}{30}.$$

RESULTS OF THE COMPUTATIONAL EXPERIMENT

To study the dynamics of near-surface dislocation loops with the use of the mathematical model (1) a program Dislocation Dynamics of Crystallographic Slip (DDCS) [8] has been developed. It implements a numerical Gear method of a variable order and an integration step [9–11], which is most suitable for the solution of the system (1). The program DDCS has an advanced user interface allowing an easy operation for researchers without a programming experience and knowledge in the field of numerical methods.

Using the program DDCS it is possible to carry out both individual calculations of the dynamics of near-surface dislocation loops and a series of calculations for the selected variable parameter of the model (for example, temperature, dislocation density, etc.) and specified limits of its change. The possibility of viewing the results of computational experiments in the graphic form and exporting data into text files has been implemented.

The program DDCS contains a database of parameter values of the mathematical model (1), obtained based on the results of experimental and theoretical data presented by different authors.

The computational experiments have been performed using the following parameter values of the mathematical model, taken from an array of experimental data proposed by different authors for lead at room temperature [12–15]: $B = 3{,}4\cdot10^{-5}$ Pa·s; $G = 7\cdot10^{9}$ Pa; $b = 3{,}5\cdot10^{-10}$ m; $\nu = 0{,}35$; $d = 8935$ kg/m^3; in calculations it is assumed that $\tau_f = 1$ MPa, $\delta = 2$ micron.

As a result of the study it has been established that the mechanical impact on a crystal leads to formation on its surfaces of closed prismatic dislocations with Burgers vector perpendicular to the bedding plane of the loop and a cylindrical slip surface, the generator of which is parallel to the Burgers vector and the guiding coincides with the dislocation loop. It has been shown that in the process of a heterogeneous nucleation the prismatic dislocation loop acquires a velocity close to the speed of sound (Fig. 1, *a*). At the near-sonic speed the dislocation loop expands on the path of about 3.6 microns, and then its velocity drops dramatically. The dislocation stops on the path of less than 3.7 microns. This pattern is observed regardless of the size of the contact spot.

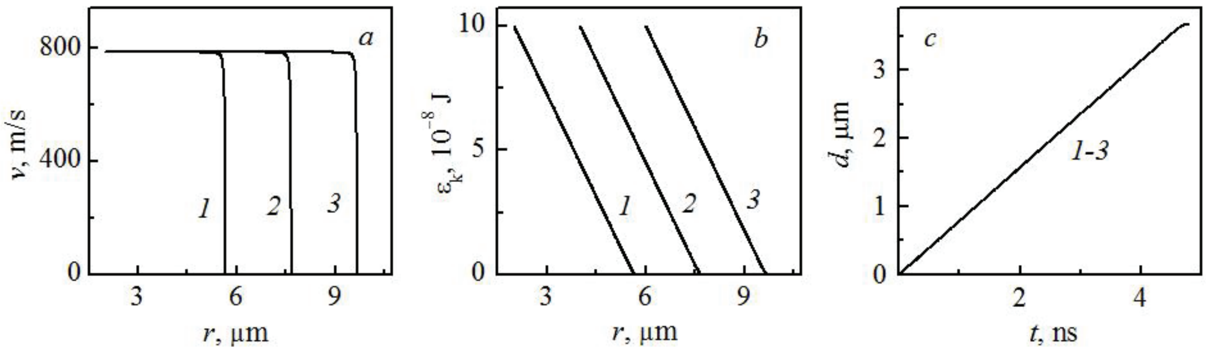

FIGURE 1. The dependence of the dislocation velocity v (a), the kinetic energy per unit length of the dislocation ε_k (b) on the dislocation path length, and the dependence of the dislocation path length r on its path time (c) with a different diameter of the contact spot, micron: 1 – 2, 2 – 4, 3 – 6

The prismatic dislocation possesses a considerable kinetic energy during its formation. In the performance of the computational experiment the values of evaluation of the initial kinetic energy have been used. As a result of the carried out study it has been shown that the kinetic energy of the dislocation loop decreases immediately after the activation, and the decrease is linear both depending on the expansion time and the path length (Fig. 1, *b*).

The diameter of the dislocation loop in the final configuration D can be calculated using the formula $D = \delta + 2 \cdot d$, where d is the path length of the prismatic dislocation. The path length of the dislocation increases linearly over time with a slight stoppage at the end of the expansion (Fig. 1, *c*). At the same value of the initial kinetic energy of the heterogeneously formed prismatic dislocation, the path time of the dislocation does not depend on the size of the contact spot and for specified parameter values of the mathematical model it is approximately 4.8 ns.

It has been established that irrespective of the dislocation density the activation of the near-surface prismatic dislocation loop occurs at a high velocity near the speed of sound in metal (Fig. 2, *a*). The dislocation retains the acquired velocity throughout the major part of the path. At the final path the stage of uniform expansion of the dislocation is replaced by the stage of rapid deceleration. The smaller the dislocation density in metal, the faster and the earlier the dislocation comes to a stop. It has been shown that the radius of the dislocation loop increases linearly throughout the entire path, except for the stage of the dislocation stoppage when its radius remains virtually unchanged (Fig. 2, *b*).

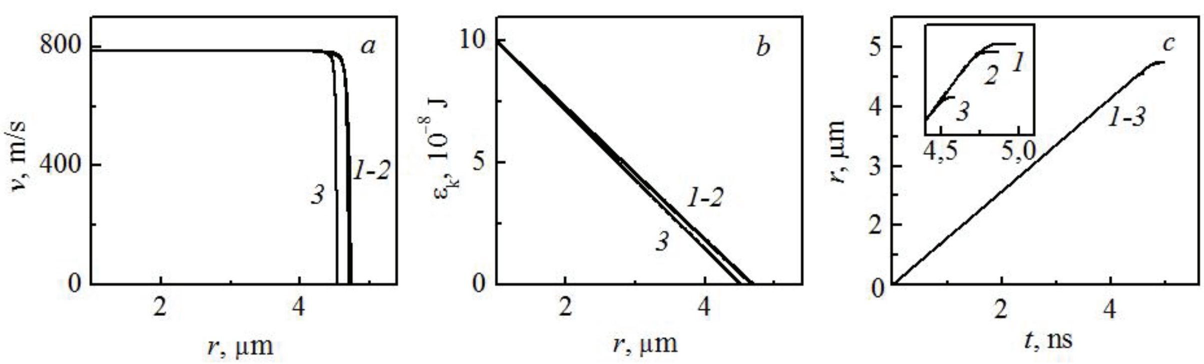

FIGURE 2. The dependence of the dislocation velocity v (a), the kinetic energy per unit length of the dislocation ε_k (b) on the dislocation path length, and the dependence of the dislocation path length r on the time of its path (c) under different dislocation densities ρ in lead, m^{-2}: 1 – 10^8, 2 – 10^{11}, 3 – 10^{13}

The radius of the dislocation loop in the final configuration slightly decreases with an increase in the density of dislocations in metal. During the expansion of the dislocation the kinetic energy per unit length of the dislocation loop decreases linearly and virtually does not depend on the dislocation density in metal (Fig. 2, *c*).

As a result of the study it has been established that the emission rate of the near-surface prismatic dislocation loop is close to the speed of sound in metal, regardless of the acquired value of kinetic energy (Fig. 3, *a*). The path length and the extension time of the prismatic dislocation loop are directly proportional to the initial kinetic energy (Fig. 3). The kinetic energy of the dislocation loop decreases linearly throughout its path. The radius of the dislocation loop increases linearly practically throughout the entire path time of the dislocation, except for a small path prior to its stoppage.

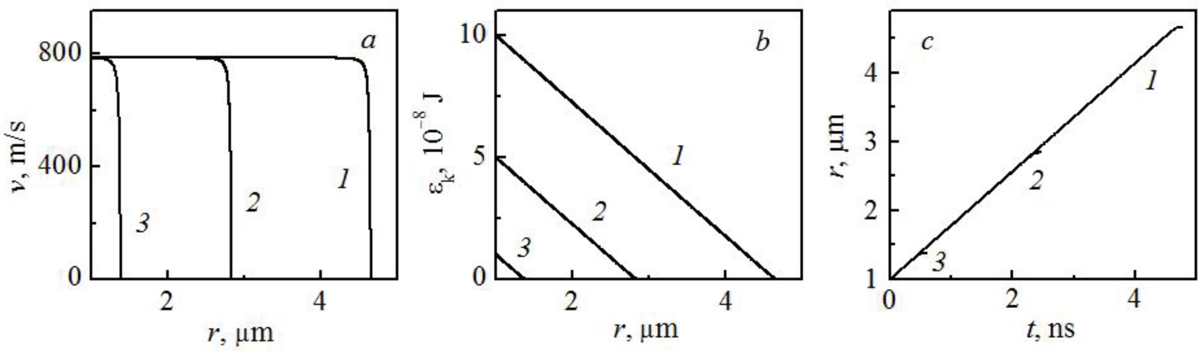

FIGURE 3. The dependence of the dislocation velocity v (*a*), the kinetic energy per unit length of the dislocation ε_k (*b*) on the dislocation path length, and the dependence of the dislocation path length r on its path time at different values of the initial kinetic energy $\varepsilon_k^{(0)}$, *J*: 1 – 10^{-7}, 2 – $5\cdot10^{-8}$, 3 – 10^{-8}

CONCLUSION

Thus, as a result of the study it has been shown that the activation of the near-surface prismatic dislocation loop occurs at a high velocity close to the speed of sound in metal, regardless of the initial value of kinetic energy, the area of the contact spot, and the density of dislocations in lead. The dislocation expands at a velocity close to the speed of sound in metal practically throughout the entire path and drops sharply at the stage of the dislocation stoppage. The kinetic energy of the prismatic dislocation loop decreases linearly throughout the path, and the radius of the dislocation loop increases linearly practically throughout the entire path, except for the stage of the dislocation stoppage.

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