Study of the Influence of Impurity and Lattice Friction on the Expansion Dynamics of Dislocation Loops in FCC Metals

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Abstract: The article presents the study on the influence of lattice and impurity friction on the expansion dynamic of dislocation loops emitted by Frank-Reid source, in nickel, copper, aluminum, and lead. A mathematical model written under the assumption that a dislocation loop expands in a homogeneous isotropic medium and is in the shape of a circle is used to carry out the study. The studies on the influence of lattice and impurity friction on the width of a dislocation cluster, the radius of the crystallographic shear zone, the number of dislocations in a dislocation cluster, and the maximum value of the velocity of the first emitted dislocation loop is carried out, and their linear relationship is shown. It is established that the maximum velocity and the path of the last emitted dislocation depend insignificantly on lattice and impurity friction, and the path of the last dislocation also depends insignificantly on metal.

Keywords: lattice and impurity friction, dislocation loop, mathematical modeling, FCC-metals, dislocation cluster.

I. INTRODUCTION

Crystallographic slip is one of the most common phenomena of the plastic form change in crystalline solids. At the present time, simulation [1]–[3] and mathematical [4], [5] modeling are widely used along with experimental methods to study the dynamics of the crystallographic slip. The objective of the given work is to study using the methods of mathematical modeling the dependence of lattice and impurity \( \tau_f \) friction on the expansion dynamics of a dislocation loop in copper, nickel, aluminum, and lead.

II. MATHEMATICAL MODEL

The mathematical model [6] was used to study the influence of lattice and impurity friction \( \tau_f \) on the expansion dynamics of the dislocation loop, written under the following assumptions: the dislocation loop has the shape of a circle in the initial configuration and during its expansion; the slip is carried out in a homogeneous isotropic medium (the continuum theory of dislocations is used [7]); the linear tension is uniform throughout the entire length of the loop; the stress associated with generation of point defects on screw and near-screw components of the dislocation loop is evenly distributed throughout the entire length of the loop.
III. Computational Experiment Results

In the implementation of the mathematical model (1) and in the study of the expansion dynamics of dislocation loops in FCC-metals the software Dislocation Dynamics of Crystallographic Slip (DDCS) was used [8]. The numerical Gear method of the variable step and order is implemented in DDCS [9], [10]. The parameter values of the mathematical model [8] obtained by different authors for lead, aluminum, nickel, and copper at room temperature (Table 1 in [8]), as well as under the stress of 23 MPa acting on the dislocation source, were used in the implementation of computational experiments.

The carried out computational experiments has shown that the dislocation velocity and the kinetic energy per unit length of the dislocation dramatically increase immediately after the emission of dislocation loop. After the negotiation of the initial path an increase in listed characteristics is replaced by a monotonous decrease. These patterns are characteristic of all dislocations emitted by one Frank-Reid dislocation source. Fig. 1 shows peculiarities of the change in time of the kinetic energy per unit length of the dislocation and the dislocation velocity for the first, middle, and the last emitted dislocation. The number of dislocations emitted at a different stress value of lattice and impurity friction is different. The middle and the last dislocation an in Fig. 1 refer to dislocations numbered, respectively, 33 and 66 (at $\tau_f = 0.1$ MPa), 23 and 47 (at $\tau_f = 1$ MPa), 15 and 30 (at $\tau_f = 2$ MPa).
Fig. 1 The dependence of current kinetic energy per unit length of the dislocation (a, c, e) and dislocation velocity (b, d, f) on its path for the 1st (curve 1), middle (2), and the last (3) dislocation loop. Stress of lattice and impurity friction 0.1 MPa (a, b), 1 MPa (c, d), 2 MPa (e, f). Nickel, room temperature.

It has been shown that an increase in the stress of lattice and impurity friction, as well as an increase in the quantity of dislocations, leads to a decrease in its path, as well as maximum values of the dislocation velocity and the kinetic energy per unit length of the dislocation loop. For each subsequent dislocation the length of the initial dislocation path decreases in absolute value, but increases in relation to the length of the entire path of the dislocation.

Patterns of the change in the dislocation loop radius can be divided into two stages – the stage of a rapid increase in the radius and the stage of the dislocation stopping, when the dislocation loop moves at a very low rate close to zero for a long time. The time of the dislocation stopping is proportional, and the time of a rapid increase in the radius is inversely proportional to the number of the emitted dislocation (Fig. 2). Therefore, the stage of dislocation stopping for the first dislocation loop takes almost a half of all time of the dislocation path, and for the last dislocation loop the stopping stage takes almost the entire time of the dislocation loop.
expansion (nearly 98%). It shall be noted that, for clarity, the value of the current radius of the last dislocation in Fig. 2 represented only for a small initial stage of its expansion.

Fig. 2. The dependence of the current dislocation radius on its path time for the 1st (curves 1-3) and the last (4-6) dislocation loop at a stress value of lattice and the impurity friction 0.1 MPa (1, 6), 1 MPa (2, 5), and 2 MPa (3, 4). Nickel, room temperature

The width of the dislocation cluster \( W \), calculated as the difference between the path of the first and the last dislocation loop, decreases linearly with an increase in the stress, lattice and impurity friction (Fig. 3a). An increase in impurity and lattice friction from 0.1 MPa to 2 MPa leads to the change in the width of the dislocation cluster in nickel in 1.5 times, in copper – by 20%, and almost by 10% in aluminum and lead. The width of a dislocation cluster in lead is about 4 times greater, in copper is almost 2 times less, and nickel is about 3 times less than in aluminum.

Fig. 3. The dependence of the dislocation cluster width \( (a) \) and the number of dislocations in the dislocation cluster \( (b) \) on the stress of lattice and the impurity friction, calculated for lead (curve 1), aluminum (2), copper (3), and nickel (4)

An increase in lattice and impurity friction from 0.1 MPa to 2 MPa leads to a decrease in the number of dislocations in the crystallographic shear zone by 20% lead, by nearly 40% in aluminum, by 25% in copper and, more than 2 times in nickel (Fig. 3b). In regards to the
absolute value, the number of dislocations in the crystallographic shear zone decreases by dislocations 5780 in lead, 540 in aluminum, 100 in copper, and 35 in nickel.

It has been in nickel an increase in the number of the emitted dislocation loop its radius in the final configuration decreases quasi-linearly in approximately 2.5 times at the value of lattice and impurity friction 0.1 MPa, and approximately in 2 times at 2 MPa (Fig. 4). Similar patterns are true for other metals under consideration. It shall be noted that the radius of the last emitted dislocation loop is practically independent of lattice and friction impurity in nickel and is approximately 25 microns, in copper – approximately 23 microns, in lead and aluminum – 20.5 microns. The dependence of the maximum radius (path length) of the first emitted dislocation loop on the value of lattice and the impurity friction has a weakly-expressed linear character (Fig. 5). A decrease in lattice and friction impurity from 2 MPa to 0.1 MPa leads to an increase in the path length of the first dislocation loop by approximately 10% in lead and aluminum, 14% in copper, and 18% in nickel.

Fig. 4. The dependence of the dislocation loop radius on its number in the dislocation cluster, calculated in nickel at a stress value of lattice and the impurity of friction 0.1 MPa (curve 1), 0.5 MPa (2), 1 MPa (3), 1.5 MPa (4), and 2 MPa (5)

The linear dependence of the maximum velocity of the dislocation loop on the dislocation number is established. Thus, in nickel the maximum velocity of the first emitted dislocation is approximately 2 times greater than the maximum velocity of the last dislocation at the value of lattice and impurity friction 0.1 MPa, and about 1.5 times greater at 2 MPa (Fig. 6). Similar patterns are true for other metals under consideration. It shall be noted that maximum velocity of the last emitted dislocation loop is practically independent of lattice and friction impurity, but is different in various metals: in nickel 43 m/s, in copper – 37 m/s, in lead – 5 m/s, and in aluminum – 85 m/s.

A decrease in lattice and impurity friction from 2 MPa to 0.1 MPa leads to an increase in the maximum velocity of the first dislocation loop emitted by the dislocation source by approximately 10% in lead and aluminum, 17% in copper, and more than 25% in nickel (Fig. 7). In regards to the absolute value, the maximum velocity in nickel, copper, and lead increases by
about 20 m/s, and by more than 100 m/s in aluminum.

Fig. 6. The dependence of the maximum velocity of the dislocation loop on its number in the dislocation cluster, calculated in nickel at a stress value of lattice and the impurity friction 0.1 MPa (curve 1), 0.5 MPa (2), 1 MPa (3), 1.5 MPa (4), and 2 MPa (5).

Fig. 7. The dependence of the maximum velocity of the first dislocation loop on the stress of lattice and impurity friction for lead (curve 1), aluminum (2), copper (3), and nickel (4).

It shall be noted that the average value of the expansion velocity of first few dislocation loops, calculated as the ratio of the dislocation path time on its motion time, is in good agreement with the experimental data [11]. In the nearest future it is planned to carry out a similar study taking into account the force of elastic interaction among all emitted dislocation loops [12], or taking into account the self-action of dislocation loops [13].

IV. CONCLUSION

The carried out study has shown that in nickel, copper, lead, and aluminum the width of the dislocation cluster, the radius of the crystallographic shear zone (equal to the radius of the first emitted dislocation loop), the number of dislocations in the dislocation cluster, and the maximum velocity of the first emitted dislocation loop have a linear inverse proportional dependence on lattice and impurity friction. It has also been revealed that the maximum velocity and the path of the last emitted dislocation is virtually independent on impurity and lattice friction, and the path of the last dislocation also depends insignificantly on metal.

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