Ultrasonics 64 (2016) 77–82

Contents lists available at ScienceDirect

Ultrasonics

journal homepage: www.elsevier.com/locate/ultras

Drift of dislocation tripoles under ultrasound influence

R.T. Murzaev [a], D.V. Bachurin [a,b,*], A.A. Nazarov [a,c]

[a] Institute for Metals Superplasticity Problems of Russian Academy of Sciences, 450001 Ufa, Russia
[b] Institute for Applied Materials – Applied Materials Physics, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany
[c] Bashkir State University, 450074 Ufa, Russia

ARTICLE INFO

Article history:
Received 26 January 2015
Received in revised form 2 July 2015
Accepted 1 August 2015
Available online 6 August 2015

Keywords:
Modeling
Ultrasound influence
Dislocation tripole
Rearrangement

ABSTRACT

Numerical simulations of dynamics of different stable dislocation tripoles under influence of monochromatic standing sound wave were performed. The basic conditions necessary for the drift and mutual rearrangements between dislocation structures were investigated. The dependence of the drift velocity of the dislocation tripoles as a function of the frequency and amplitude of the external influence was obtained. The results of the work can be useful in analysis of motion and self-organization of dislocation structure under ultrasound influence.

1. Introduction

Significant changes of the dislocation structure may occur in crystalline materials under the influence of alternating loading and/or ultrasonic waves [1–6]. These changes at high amplitudes result in an intensive generation of dislocations and formation of a cellular structure [6–9], nucleation of fatigue cracks and fracture [10] and hardening or softening of the material [3,11]. Nanostructuring of the surface was revealed under intensive ultrasonic treatment [12–14]. On the other hand, a structural relaxation of non-equilibrium materials takes place under ultrasonic impact with mediate amplitudes. An increase of thermal stability of amorphous state together with the structural relaxation and reduction of the free volume was observed in metallic glasses [15]. Ultrasonic exposure with amplitudes comparable to the yield stress led to the hardening of polycrystalline hafnium in the annealed state and loss of the strength after deformation, which is related to the generation of defects and relaxation of internal stresses, respectively [16].

Relaxation of non-equilibrium grain boundaries and an increase of thermal stability of the microstructure were revealed in nanocrystalline materials prepared by severe plastic deformation method [17]. Ultrasonic treatment led to a significant increase of plasticity of these materials at the retaining or even improving of the ultimate strength [18,19]. Ultrasound impact on the predeformed nanocrystalline structure of ZrNb alloy invoked dynamic recovery and significant relaxation of internal stresses at maintaining nanostructured morphology and improved uniformity of the structure [20]. Understanding of the structural changing occurring under the ultrasonic impact of different amplitudes and their influence on the properties of materials requires the study of the mechanisms of formation and dynamics of elementary dislocation structures such as dislocation dipoles and multipoles.

In experimental studies it is possible to determine empirically the initial and the final positions of the dislocations, while the peculiarities of the motion of dislocations during ultrasonic treatment are undetectable. Therefore, a theoretical study together with computer simulation are the most convenient way to study the dynamics of dislocation systems. Analytical results for the interaction of an elastic wave with a single dislocation [21], a random distribution of dislocations [22,23] and arrangement of dislocation walls [24–26] were obtained. Simulation of the motion of a screw dislocation in the field of the fixed dislocation with the same Burgers vector was performed by Lomakin [27], and the behavior of a dislocation dipole (two edge dislocations with opposite signs of Burgers vector) in an ultrasonic field was studied in Refs. [28–30]. Note, that the authors [27–30] did not detect any translational motion of the studied dislocation structures.

The movement of a dislocation tripole under the influence of oscillating stresses was considered in the paper [31]. The authors have revealed the occurrence of the tripole's drift, i.e. the translational motion of its centre of mass. The velocity of this tripole was found to be a function of the amplitude and the frequency of

* Corresponding author at: Institute for Applied Materials – Applied Materials Physics, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany. Tel.: +49 721 608 23639; fax: +49 721 608 24567.
E-mail address: dmitry.bachurin@kit.edu (D.V. Bachurin).

http://dx.doi.org/10.1016/j.ultras.2015.08.001
0041-624X/

the external stress. In some cases, depending on the initial conditions, at low frequencies two different stationary solutions were found, which correspond to different drift velocities. In the first solution at a certain value of the frequency a drastic increase of the drift velocity was observed, while in the second solution the drift velocity sharply reduces to zero. The reason of such behavior in Ref. [31] has not been fully understood.

The effect of alternating loading on the plastic deformation of a monocrystal together with the processes of dislocation nucleation and their motion was studied by Blagoveshchenskii and Panin [32] by means of computer simulations. Redistribution of dislocations under ultrasound influence followed by the formation of the ordered dislocation ensembles with the distinct cellular structure was found in Refs. [9,33]. Self-organization of such dislocation structures occurred due to the motion (gliding) both single and coupled into the multipoles dislocations.

The aim of this work is numerical simulation of translational movement of stable triple dislocation configurations under influence of periodic alternating stress with the zero average value.

2. Theoretical background

Velocity of a straight infinite edge dislocation is described with the relation:

$$V = B\,|\tau|^m \cdot \mathrm{sign}(\tau). \tag{1}$$

Here τ is a total shear stress in the dislocation glide plane in the direction of Burgers vector; B is a mobility factor; m is a constant which is equal to several units at mediate shear stresses. As it follows from expression (1), in the case of symmetrical cyclic loading the dislocation exhibits symmetric oscillations with respect to a certain equilibrium point.

Shear stress for an edge dislocation with Burgers vector of $\vec{b}(b,0,0)$ in the plane parallel to its glide plane can be written as

$$\tau(x,y) = Db\cdot\frac{x(x^2-y^2)}{(x^2+y^2)^2}, \tag{2}$$

where $D = G/2\pi(1-\nu)$; G is a shear modulus and ν is a Poisson's coefficient [34]. Analysis of expression (2) shows, that two dislocations with the parallel glide planes at certain positions do not interact with each other (interaction force is equal to zero) and may form two different coupled stable configurations. One of them is composed of dislocations of the same sign and is a fragment of the dislocation wall, the second made up of two dislocations of the opposite signs of Burgers vector is a dislocation dipole.

Similarly, there are stable systems of three coupled dislocations. In these systems all of the dislocations may be of the same sign or one dislocation may have a sign opposite to that of the other two dislocations. In the latter case we deal with dislocation tripoles. During plastic deformation such tripoles may be formed by impingement of individual dislocations on the immobile dipoles. The structure of the dislocation tripoles is very manifold.

3. Model

Let us suppose that the dislocations in the tripole exhibit an external alternating loading $\tau(t)$. We assume that this field is uniform within the tripole. In other words, the system experiences the effect of a standing sound wave with a wavelength much longer than the possible amplitudes of motion of the dislocations. Velocity of the dislocations is also considered to be small compared to the velocity of sound in the material, i.e. we ignore the relativistic effects. We also neglect the effect of crystallographic orientation of the sample on the dislocation dynamics as well as the influence of various kinds of impurity atoms and other defects. We consider only gliding of the dislocations without any climbing process.

Let us choose x-axis as a direction of dislocation glide. x_1, x_2 and x_3 denote the displacement of the first, second and third dislocations from their equilibrium positions. τ_{ij} is a shear stress of i-th dislocation in the position of j-th dislocation. The function τ_{ij} can be evaluated using formula (2). For simplicity, we assume that m is an integer odd number. The system of equations of motion of dislocation tripole can be written in the following way:

$$\begin{aligned}
\frac{dx_1}{dt} &= B(S_1\cdot\tau(t) + \tau_{31}(x_1-x_3, y_1-y_3) + \tau_{21}(x_1-x_2, y_1-y_2))^m\\
\frac{dx_2}{dt} &= B(S_2\cdot\tau(t) + \tau_{23}(x_2-x_3, y_2-y_3) - \tau_{21}(x_1-x_2, y_1-y_2))^m\\
\frac{dx_3}{dt} &= B(S_3\cdot\tau(t) - \tau_{32}(x_2-x_3, y_2-y_3) - \tau_{31}(x_1-x_3, y_1-y_3))^m.
\end{aligned} \tag{3}$$

Here $S_i = \pm 1$ depends on the sign of the dislocation; $\tau(t)$ is an external stress, which is assumed to vary sinusoidally as $\tau(t) = \tau_0 \sin \omega t$, where τ_0 and ω are the amplitude and the frequency of the external load, respectively. Here the phase shift is supposed to be zero, which corresponds to a standing wave. The first argument of the function τ_{ij} contains only the difference $(x_i - x_j)$, since the shear stress of an edge dislocation at some point and in a given plane depends only on the distance to this point along the x-axis. It is also taken into account that $\tau_{ji} = \tau_{ij}$.

For the numerical solution the system of Eq. (3) can be rewritten in dimensionless variables: $\tilde{t} = t\cdot\omega$ for time and $\tilde{x} = x\cdot\omega/B\tau_0^m$ for the distance. Let us represent the stresses of interaction of dislocations through the universal function that depends only on the coordinates:

$$\tau_{ij}(x_j - x_i, y_j - y_i) = Dbf_{ij}(x_j - x_i, y_j - y_i), \tag{4}$$

where

$$f(x,y) = \frac{x(x^2-y^2)}{(x^2+y^2)^2}. \tag{5}$$

After elementary transformations the system (3) can be written as

$$\begin{aligned}
\frac{d\tilde{x}_1}{d\tilde{t}} &= \left(S_1\sin(\tilde{t}) + \frac{Db\omega}{B\tau_0^{m+1}}[(f_{31}(\tilde{x}_1-\tilde{x}_3, \tilde{y}_1-\tilde{y}_3) + f_{21}(\tilde{x}_1-\tilde{x}_2, \tilde{y}_1-\tilde{y}_2)]\right)^m\\
\frac{d\tilde{x}_2}{d\tilde{t}} &= \left(S_2\sin(\tilde{t}) + \frac{Db\omega}{B\tau_0^{m+1}}[(f_{23}(\tilde{x}_2-\tilde{x}_3, \tilde{y}_2-\tilde{y}_3) - f_{21}(\tilde{x}_1-\tilde{x}_2, \tilde{y}_1-\tilde{y}_2)]\right)^m\\
\frac{d\tilde{x}_3}{d\tilde{t}} &= \left(S_3\sin(\tilde{t}) - \frac{Db\omega}{B\tau_0^{m+1}}[(f_{32}(\tilde{x}_2-\tilde{x}_3, \tilde{y}_2-\tilde{y}_3) + f_{31}(\tilde{x}_1-\tilde{x}_3, \tilde{y}_1-\tilde{y}_3)]\right)^m.
\end{aligned} \tag{6}$$

Each equation of the system (6) written in the dimensionless coordinates depends on the single parameter $K = Db\omega/B\tau_0^{m+1}$, which is a contribution of interaction between dislocations into the drift velocity of dislocation tripole. An increase of K corresponds to simultaneous increase of frequency ω and/or a decrease of amplitude τ_0.

The magnitude of the drift velocity of dislocation tripole in dimensionless coordinates is

$$\tilde{V} = \frac{1}{3}\cdot\overline{\left(\frac{d\tilde{x}_1}{d\tilde{t}} + \frac{d\tilde{x}_2}{d\tilde{t}} + \frac{d\tilde{x}_3}{d\tilde{t}}\right)}. \tag{7}$$

where the bar denotes averaging over the entire loading period. In particular, as it follows from the system (6), when $m = 1$, the drift velocity of the centre of mass of tripole is $V = \pm B\tau(t)/3 = 0$, which corresponds well to the case of motion of dislocations in copper