



Drift of dislocation tripoles under ultrasound influence



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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.

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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 pre-deformed 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

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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:

$$V = B |\tau|^m \cdot \text{sign}(\tau). \quad (1)$$

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

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

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 triplets. During plastic deformation such triplets may be formed by impingement of individual dislocations on the immobile dipoles. The structure of the dislocation triplets is very manifold.

3. Model

Let us suppose that the dislocations in the triplet exhibit an external alternating loading $\tau(t)$. We assume that this field is uniform within the triplet. 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 triplet can be written in the following way:

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

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:

$$\tau_{ij}(x_j - x_i, y_j - y_i) = Db f_{ij}(x_j - x_i, y_j - y_i), \quad (4)$$

where

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

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

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

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 triplet. 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 triplet in dimensionless coordinates is

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

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 triplet is $V = \pm B\tau(t)/3 = 0$, which corresponds well to the case of motion of dislocations in copper

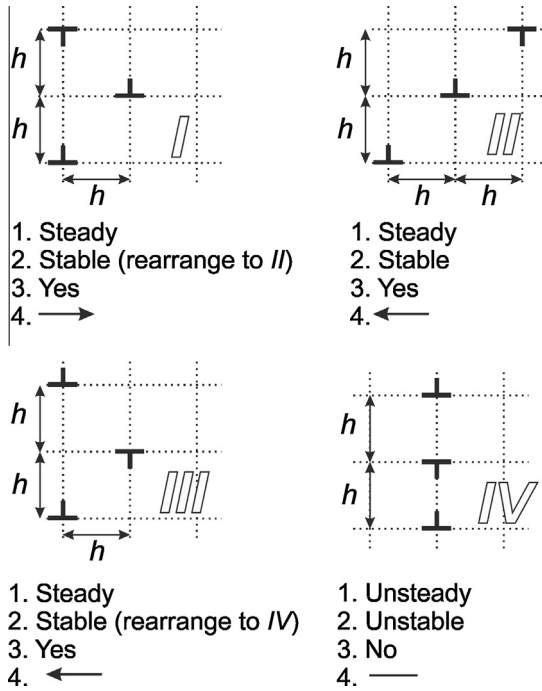


Fig. 1. Initial structure of the tripole configurations considered in the present paper. The numbers below the plots mean the following: (1) steadiness of the structure (without ultrasonic treatment); (2) stability of the structure (after ultrasonic treatment); (3) presence (yes/no) and (4) direction (\rightarrow / \leftarrow) of the drift, as well as the possible rearrangements.

[35]. That is, a nonlinearity of the dependence of $V(\tau)$ in Eq. (1) is a necessary condition for the existence of the drift effect [31].

The system of Eq. (6) was solved numerically using Runge-Kutta fourth order method. The following parameters of the model and initial conditions were used. Since the non-linearity of the relation (1) is a necessary condition for the drift, the constant m was chosen to be equal to 3. This relation describes quite well the dependence of the dislocation velocity vs. stress in α -iron at room temperature [35]. It should be noted that any other value of the constant m (excluding $m = 1$) will affect only the dislocation velocity and have no influence on the qualitative characteristics of the drift and rearrangements of dislocation tripoles. Therefore, in this study, the choice of the constant m was related to a convenience of calculations. Integration step was selected to be $dt = 2\pi \cdot 0.0001/\omega$. In order to estimate the coefficient K , the following values of the fundamental parameters for α -iron were used: $B = 1$, $b = 2.482 \text{ \AA}$, $G = 82 \text{ GPa}$, $\nu = 0.29$. For ease of calculation it was supposed that the dimensionless distance between the dislocations $\tilde{h} = 1$. At the initial moment of time $t = 0$ the dislocations in the tripole are at the positions as indicated in Fig. 1 and have zero velocities. At $t = 0$ the effect of the oscillating stresses is turned on.

4. Results

We have investigated 16 different tripole configurations and only four of them were found to be stable and three of them were mobile under ultrasonic influence. All other dislocation systems were either immobile, or after a certain transient period rearrange into these three structures. Hereinafter we will focus on study of a behavior of these three stable mobile dislocation tripole configurations denoted as I, II and III (see Fig. 1).

After application of the external stress a steady-state quasi-periodic motion of dislocation tripoles I, II and III in the x -direction with a frequency equal to the frequency of the external applied stress is observed. Since all considered tripoles consist of

one negative and two positive dislocations (see Fig. 1), the displacement in one direction is not compensated by the displacement in the opposite direction, which leads to a non-zero drift velocity.

A detailed analysis shows that the mobile tripoles I, II and III have a phase shift between the oscillations of two positive and one negative dislocation, which is somewhat different from π . This shift can also be related to the unequal number of positive and negative dislocations in the tripoles. Note that the similar phase shift between the oscillations of dislocations of different sign for immobile tripole is equal to π .

Fig. 2 presents the dependence of the drift velocity \tilde{V} for tripoles I, II and III on the coefficient $1/K$. The velocity was calculated using formula (7) and corresponds to the slope of the gain envelope of a wave packet. As seen, the curves for all three cases have a characteristic peak, while tripole II at larger values of $1/K$ has a second less pronounced peak.

The drift of tripole I is observed only in a relatively narrow interval of $1/K$ (from 0 to 0.41). Thereafter it rearranges into the configuration II, which is the only configuration studied in this paper that can exist and be mobile at high amplitudes of ultrasound influence ($1/K > 1.03$).

Fig. 3a demonstrates the abscissas x_i of the dislocations in tripole I as functions of time calculated for the value of $1/K \approx 0.41$. It is seen that the amplitude of the oscillations of each dislocation changes during the rearrangement $I \rightarrow II$, however their phase does not. The slope of the gain envelope of the wave packet to the abscissa axis indicates the presence of a drift. Thus, tripole I moves along the positive direction of the x -axis and after rearrangement into the configuration II the direction of the drift is changed to the opposite. The rearrangement $I \rightarrow II$ is accompanied by an abrupt increase of the drift velocity (shown with the arrow in Fig. 2).

In contrast to the structure I, tripole III is mobile in a wider range of values of the coefficient $1/K$ (from 0 to 1.03). At $1/K \approx 1.03$ it rearranges into the configuration IV, which is immobile (see Fig. 2). Fig. 3b shows that the rearrangement $III \rightarrow IV$ is gradual. After a certain period of time the slope of the gain envelope to the x -axis becomes equal to zero, which indicates an absence of the drift of tripole IV. In contrast to the previous case, no change of both the amplitude of oscillations and the phase during rearrangement is observed (see Fig. 3b). Dislocation tripole IV is unstable at low amplitudes of ultrasound influence and rearranges into the configuration III, while at higher values of $1/K$, when the amplitude of oscillation is comparable with the distance between dislocations h , it is in a metastable state.

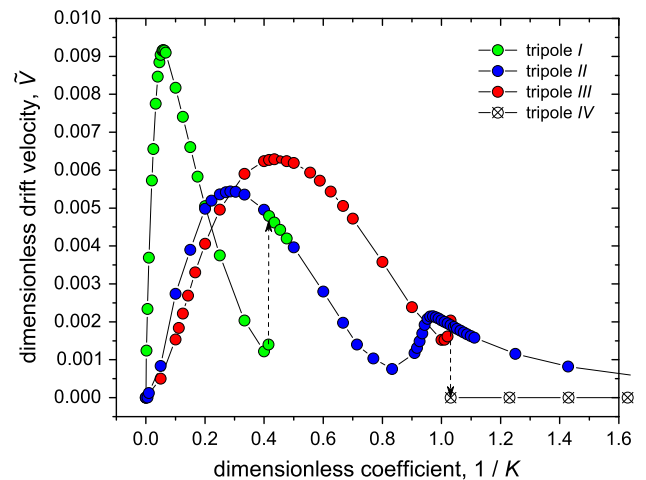


Fig. 2. The drift velocity \tilde{V} for the investigated dislocation tripoles as a function of the parameter $1/K$. The rearrangements $I \rightarrow II$ and $III \rightarrow IV$ are shown with the arrows.

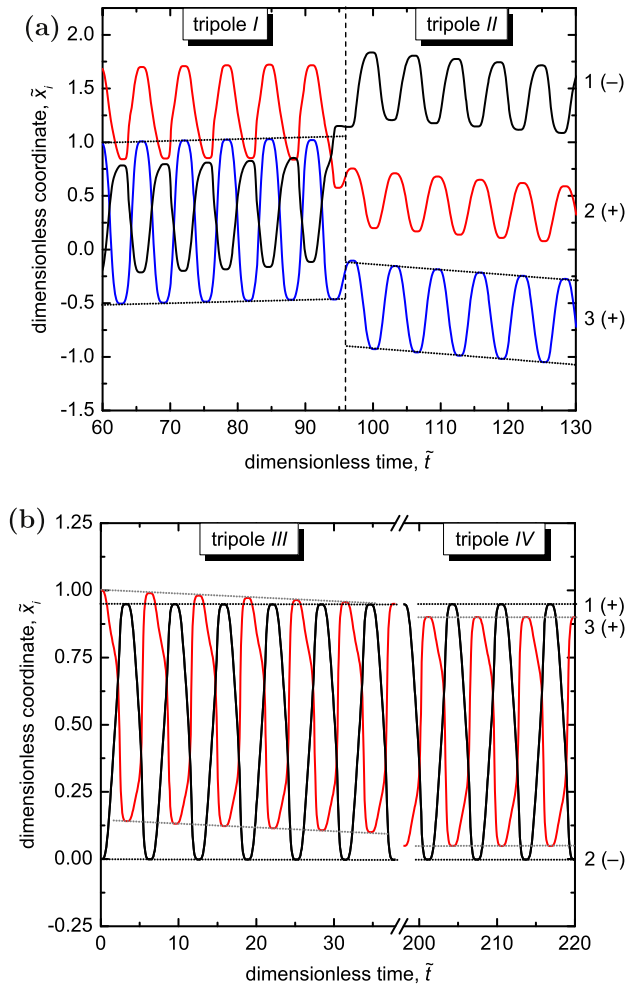


Fig. 3. Abscissas of each of the three dislocations included in tripoles (a) I and (b) III as functions of time. The sign of the dislocation in the tripole are shown in parentheses at the right side. The vertical dashed line in (a) shows the moment of rearrangement. The dotted lines are the gain envelope of the wave packets.

The rearrangements of one dislocation tripole into the other can be easily explained by calculation of the interaction energy of the rearranging dislocation with the two other dislocations within the tripole configuration. The elastic energy of such system can be calculated as the work necessary to move one dislocation along the x -direction (glide plane) at an infinite distance from the other two dislocations, which is considered to be immobile. Since the shear component of the stress field of a single dislocation decreases inversely proportional to the distance from it, then the integral (work) diverges at infinity. Therefore it is convenient to deal not with the absolute energy of the system, but with a relative (or excess) energy, correlating it with the energy system in the global minimum, i.e. $\Delta E = E_0 - E_{min}$.

Dislocation 1 in tripole I is stable and is in a local energy minimum (see Fig. 4a). However, with increasing of the amplitude of oscillation the dislocation 1 can overcome the energy barrier and move to the point with the abscissa $\tilde{x}_1 = 2$. At this position, corresponding to tripole configuration II, the dislocation 1 has the lowest energy. As seen in Fig. 4a, tripole II is more stable than tripole I.

Fig. 4b shows that dislocation 2 in tripole IV is in an unstable equilibrium point and even at small deviations this dislocation can easily displace into the point $\tilde{x}_2 = 1$ (i.e. rearrange into tripole configuration III), or to the point which is symmetric to it with respect to ordinates axis, i.e. $\tilde{x}_2 = -1$. The direction of the rearrangement depends on which side the dislocation 2 is deflected

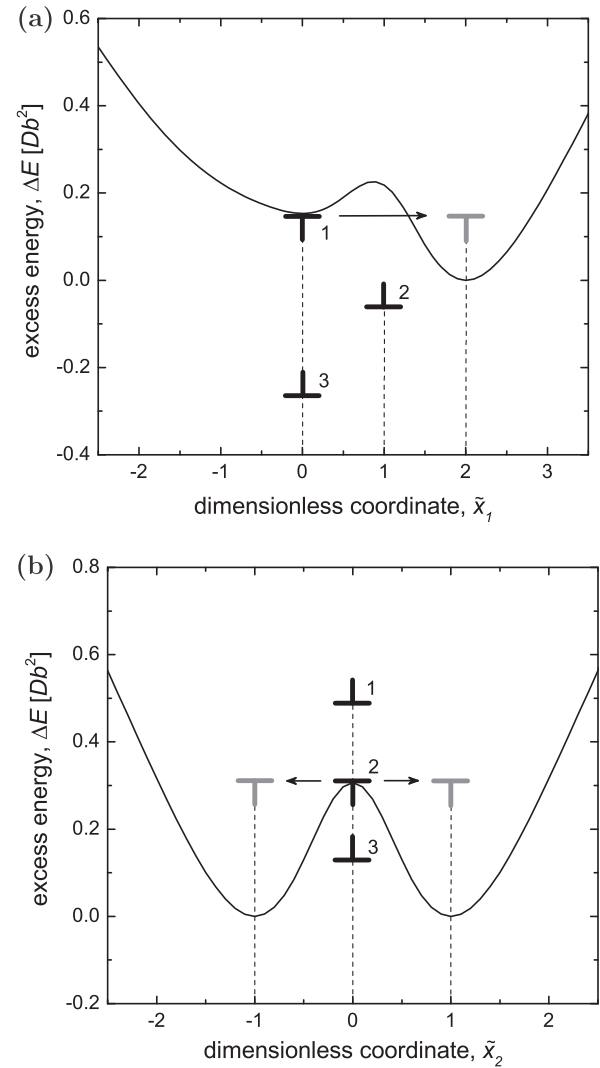


Fig. 4. Relative elastic energy as a function of the position of (a) dislocation 1 during the rearrangement I → II and (b) dislocation 2 during the rearrangement III → IV. The arrows show the corresponding displacements of the dislocation.

at the initial moment of time. Note that the rearrangement III → IV is possible only with high-amplitude fluctuations of the dislocations, when the amplitude becomes comparable with the distance between dislocations h . This is due to the fact that the fluctuation energy becomes higher than the potential barrier (see Fig. 4b) and dislocation 2 moves from the position $\tilde{x}_2 = 1$, which corresponds to the minimum of potential energy, to the position $\tilde{x}_2 = 0$.

5. Discussion

Considered stable and mobile dislocation tripoles may rearrange into the more stable configurations corresponding to the lower potential energy. Usually this is accompanied by the displacement of one dislocation and can be explained by the calculation of the elastic energy of the rearranging dislocation within the tripole.

Based on the analysis of dynamics of the tripole configurations we can formulate the main criterion of their drift under the influence of the alternating load: if the coordinates of the centres of mass of positive and negative dislocations within the tripole do

not coincide, this tripole is mobile. Otherwise, the tripole is immobile. Systems consisting of the dislocations of the same sign are immobile in the field of a standing sound wave. The same applies to dislocation dipoles and is in agreement with previous calculations [27–30]. It should be noted that such systems including fragments of dislocation walls may drift under the influence of a travelling wave [36].

Either gradual or abrupt changes of the drift velocity in both the magnitude and the direction may occur during rearrangement of one tripole configuration to the other. The rule defining the direction of the drift follows directly from the above-mentioned criteria. Namely, if the abscissa of the centre of mass of two positive dislocations is located more to the left than that of the negative dislocation (as in the case of tripoles II and III), then this tripole drifts leftwards. Otherwise (configuration I), tripole moves rightwards. Thus, the mutual positions of the centres of mass of positive and negative dislocations completely determine the direction of the tripole's drift. A separate study has shown, that if the dislocation configurations I, II and III are mirrored relative to the vertical y -axis, then the direction of their drift changes to the opposite direction to that indicated in Fig. 1.

As a hypothesis, the formulated mobility criterion of dislocation tripoles can be generalized for more complex multipole dislocation configurations for materials with the constant $m > 1$. Namely, it can be supposed, that if such dislocation structures obtain any asymmetry in the location of the centres of mass of positive and negative dislocations, then under the influence of standing sound waves these structures will drift.

The obtained dependence of the drift velocity on the parameter $1/K$ for tripole III exactly coincides with the results of Ref. [31]. However, the authors [31] do not associate the observed velocity reduction to zero (the first solution) with the rearrangement of the structure of tripoles (rearrangement III \rightarrow IV), when tripole IV is immobile due to the coincidence of the centres of mass of the dislocations of opposite sign. In addition, for each tripole configuration we have found the only stationary solution with the corresponding non-zero drift velocity. The existence of the second solution found in Ref. [31] is related to the initial phase shift in the movement of the dislocations of opposite sign, which corresponds to a travelling sound wave and lays beyond the scope of this paper.

The drift of tripole and multipole configurations under ultrasound exposure is an elementary act of self-organization of dislocation structure described in Ref. [9] (see Fig. 1). This redistribution of dislocations results in formation of dynamically ordered dislocation structure, which is observed also experimentally in single crystals of magnesium oxide and zinc [9]. Note, that such systems of structural defects do not have long-range stress fields [6].

The drift of dislocation configurations under the influence ultrasound can have a significant impact on the development of inhomogeneities in various dislocation substructures, for example, can lead to relaxation of residual defect structure in deformed polycrystals. The results of the paper can be useful in analysis of motion and self-organization of dislocation structure occurring under ultrasound influence. Since the ultrasound treatment is an additional tool for controlling the structure and properties of materials, then combination of annealing and ultrasonic exposure gives a possibility to improve mechanical properties of materials [18,37].

6. Conclusions

The dynamics of different dislocation tripoles interacting with a standing acoustic wave in a wide interval of values of the coefficient $1/K$ was studied. Main conclusions can be formulated as follows:

1. There are tripole dislocation configurations which can move under ultrasound influence.
2. Three different stable mobile configurations of dislocation tripoles were found. One stationary solution with a non-zero drift velocity corresponds to each configuration.
3. The drift of the dislocation tripole (and multipole in the general case) occurs when the centres of mass of positive and negative dislocations in their statically equilibrium configuration do not coincide. The direction of the tripole's drift is also determined by the mutual arrangement of the centres of mass of the dislocations of opposite sign.
4. The dynamics of the dislocation tripole is completely determined by its structure.

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