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## Propagation of a switching wave when intense plastic deformation is applied by torsion

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Received August 16, 2025

Revised October 1, 2025

Accepted October 18, 2025

The shape of the kink is studied when intense plastic deformation is applied by torsion. It is shown that the process of transition to a stationary state in a two-component copper solution is oscillatory. The behavior of the rates of change in the densities of edge and screw dislocations as functions of deformation is revealed, which leads to a spiral dependence of these dependencies

**Keywords:** kink, dislocations, order parameter, phenomenological Landau theory, Lifshitz invariants, intense plastic deformation by torsion, self-similar substitution.

DOI: 10.61011/PSS.2025.10.62647.89-25

### 1. Introduction

Industrial materials often undergo high breaking loads. It is therefore relevant to study the formation of their properties when these materials are subjected to the severe megaplastic deformation. Such loads may rise at a low or high rate. In the latter case, a pulse wave in the form of a kink may occur. This process is an autowave itself and represents the simplest topological soliton. The kink looks like a wall separating two space areas that have different values of a certain magnitude. Obviously, after passing the kink, an equilibrium state is expected to be set. However, if the external pulse is strong enough, the system, regardless of its initial state, will switch to a stationary state that was discovered in [1–5] during the study of two-component copper solutions impacted by a severe plastic torsional deformation (SPTD).

Autowave processes are widespread in nature. In particular, these are the waves in Belousov–Zhabotinsky reaction [6], in biological tissues [7,8], interphase boundaries [9,10]; localized strongly non-equilibrium states in the homogeneous dissipative structures [11,12]. Currently, the kink dynamics is studied in sufficient detail for various processes based on the sine-Gordon equation. In [13], the dynamics of a kink in a spatially inhomogeneous periodic potential environment and with a single point impurity is studied. The analytical velocity-time dependences of a kink moving under the action of a homogeneous unsteady external force in a dissipation medium are investigated [14] and the cases of a harmonically time-dependent external force and a stepwise time-dependent force are reviewed. It was shown that for approximation of a „non-deformable

kink“ the impurity acts like an attracting potential, therefore, the solitons may be localized and radiate [15].

In the case of „approximation of a deformable kink“, in addition to the oscillatory motion of the kink at the potential created by the impurity, the effects of kink deformation (e.g., a strong change in its shape) occur, having a resonant character [15]. The possibility of exciting an impurity mode during kink scattering was also taken into account, leading to a significant change in the results of the kink dynamics [16]. An interesting effect is also observed here — kink reflection by an attractive impurity due to the resonant energy exchange between the translational kink mode and the impurity mode.

We also considered the case of many delta-shaped „point impurities“ which are of interest for some physical applications [17], and even the case of spatial modulation of a periodic harmonic potential [18]. It should be noted that the influence of large perturbations, in general, can be carried out only using numerical methods [19,20]. In paper [21] it was demonstrated that perturbed sine-Gordon equation has a good quality in describing the dynamics and interaction of kinks with the topological charges  $S = \pm 1$  in the nematic liquid crystals (NLC).

In addition, the dependence of the umklapp wave velocity on the non-locality parameter of the medium was studied [22], subsonic and supersonic modes of wave motion were considered. Conditions of stability of kink and anti-kink in „medium–source“ systems were studied [23]. It should be noted that the study of the kink shape using Landau’s phenomenological theory in a general form in the two-component copper compounds under the action of SPTD neglecting the behavior of dislocations was carried out in [24].

The kink models discussed earlier did not take into account the presence of dynamic subsystems interacting with each other in real physical compounds, in particular, various kinds of dislocations that are critical in phase transitions. In this paper, which is a continuation of a series of papers on the study of SPTD effect on the two-component copper solutions (see reviews of [1,2]), an attempt is made to fill this gap using self-similar solutions of the Landau–Khalatnikov system of equations. It should be emphasized that experimental data confirming the conclusions of this article are currently missing, and the theoretical results obtained serve as the basis for an appropriate experiment.

## 2. Theory

As shown in papers [2,25], Landau's phenomenological theory satisfactorily describes the processes occurring in the two-component solutions. This is due to the fact that in theory a solid is represented as a continuous continuum. However, the symmetry of the problem is taken into account when choosing the appropriate order parameters. Based on Landau phenomenological theory, the non-equilibrium thermodynamic potential to describe the kink scattering when SPTD is applied along  $OZ$  axis, is expressed as

$$\begin{aligned} \Phi = & -\frac{\alpha_1}{2} q^2 + \frac{\alpha_2}{4} q^4 + \frac{\alpha_3}{6} q^6 + \beta_1 \varphi_1 + \frac{\beta_2}{2} \varphi_1^2 + \frac{\beta_3}{3} \varphi_1^3 \\ & + \frac{\beta_4}{4} \varphi_1^4 + \beta_5 \left( \frac{\partial \varphi_1}{\partial z} \right)^2 + \omega_1 \varphi_2 + \frac{\omega_2}{2} \varphi_2^2 + M(N)^2 \frac{\omega_3}{3} \varphi_2^3 \\ & + \frac{\omega_4}{4} \varphi_2^4 + M(N)^2 \omega_3 \left( \frac{\partial \varphi_2}{\partial z} \right)^2 + \delta_1 q^2 \varphi_1 + \delta_2 q^2 \varphi_2 \\ & + \delta_3 \varphi_1 \varphi_2 + \gamma_1 M(N)^s \left( q_x \frac{\partial q_y}{\partial z} - q_y \frac{\partial q_x}{\partial z} \right) \\ & + \gamma_2 M(N)^r \left[ \left( \frac{\partial q_x}{\partial z} \right)^2 + \left( \frac{\partial q_y}{\partial z} \right)^2 \right], \end{aligned} \quad (1)$$

where  $\alpha_i$  ( $i = 1-3$ ),  $\beta_i$  ( $i = 1-5$ ),  $\omega_i$  ( $i = 1-5$ ),  $\delta_i$  ( $i = 1-3$ ),  $\gamma_i$  ( $i = 1-2$ ) — phenomenological parameters,  $\mathbf{q}$  [m] — vector structural order parameter (OP), defined as a linear combination of the lattice cell's atoms shifts and transformed using some irreducible representation of a crystal symmetry group,  $q_x, q_y, q_z$  — components of vector structural OP,  $\varphi_1, \varphi_2$  [ $\text{m}^{-2}$ ] — densities of the near-band-edge and screw dislocations, i.e. total length of appropriate dislocations per unit of volume,  $N$  — number of turns,  $r-s = 4$  ( $r = 6, s = 2$ ) [2],  $M(N)$  [ $\text{N} \cdot \text{m}$ ] — torsion moment directed along  $OZ$  axis. Due to this moment, a spatial heterogeneity of the crystal structure arises, described by derivatives of the components of the structural OP. In addition, there is a heterogeneity of dislocation distribution densities. The competition of the last two terms with derivatives of the structural OP leads to the appearance of a

helical axis of symmetry, as well as a spiral distribution of the structural OP and dislocation densities [2]. The first of these two terms, made up of Lifshitz invariants, may be zero in crystals of some symmetry, but when applying SPTD, when the symmetry decreases, it will be different from zero. It is this event that explains the appearance of multiplier  $M(N)^2$  in the last two terms of the expression (1). As mentioned above, the density  $\varphi_2$  delineates the screw dislocation. In this problem it is supposed that  $\varphi_2 \neq 0$  only when SPTD is applied. Hence,  $\omega_1 = 0$ ,  $\omega_3 < 0$  and the appropriate term has  $M(N)^2$  as a multiplier. In addition, a similar multiplier contains a term with a spatial derivative of  $\varphi_2$ , since there is no screw dislocation at  $M(0) = 0$ . It should be stressed that when SPTD is applied along  $OZ$  axis, the vector of structural OP when moving along  $OZ$  rotates around this axis i.e. the components  $q_x, q_y$  change, whereas  $q_z$  remains constant under the unchanged moment. However, the modulus of the structural OP and its components depend on the magnitude of the applied moment.

Although dislocations in real FCC metals usually have a mixed character and are often associated with stacking faults, within the framework of Landau's phenomenological theory we will limit ourselves to considering the near-band-edge and screw components. At the same time, since dislocations interact with each other locally at the intersections of their dislocation lines (kernel), the total percentage of the end or screw dislocations is critical, regardless of whether these dislocations are composite or pure. For the same reason, in the phenomenological approximation, it does not matter whether they are infinite or form loops. Partial dislocations are also effectively taken into account here, since the density of dislocations of one type or another varies continuously, and the presence of partial dislocations will lead to some (small) change in the density of dislocations of the type to which this partial dislocation is closest in nature.

Let us consider the kink dynamics using Landau–Khalatnikov system of differential equations for vector and scalar OP components

$$\frac{\partial q_i}{\partial t} = -\chi_i \frac{\delta \Phi}{\delta q_i}, \quad \frac{\partial \varphi_j}{\partial t} = -\chi_j \frac{\delta \Phi}{\delta \varphi_j}, \quad (2)$$

where  $i = x, y, j = 1, 2$ ,

$$\begin{aligned} \frac{\delta \Phi}{\delta q_i} &= \sum_k^n (-1)^k \frac{d^k}{dz^k} \frac{\partial \Phi}{\partial \left( \frac{d^k q_i}{dz^k} \right)}, \\ \frac{\delta \Phi}{\delta \varphi_j} &= \sum_k^n (-1)^k \frac{d^k}{dz^k} \frac{\partial \Phi}{\partial \left( \frac{d^k \varphi_j}{dz^k} \right)} \end{aligned} \quad (3)$$

— functional derivatives,  $t$  — time,  $\chi$  — matrix kinetic coefficient characterizing the rate of relaxation of the system

to the equilibrium state. By substituting (3) in (2) we obtain

$$\left\{ \begin{aligned} \frac{\partial q_x}{\partial t} &= -\chi_x \left[ q_x(-\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta_2 \varphi_2) \right. \\ &\quad \left. + 2\gamma_1 M(N)^r \frac{\partial q_y}{\partial z} - 2\gamma_2 M(N)^s \frac{\partial^2 q_x}{\partial z^2} \right], \\ \frac{\partial q_y}{\partial t} &= -\chi_y \left[ q_y(-\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta_2 \varphi_2) \right. \\ &\quad \left. - 2\gamma_1 M(N)^r \frac{\partial q_x}{\partial z} - 2\gamma_2 M(N)^s \frac{\partial^2 q_y}{\partial z^2} \right], \\ \frac{\partial \varphi_1}{\partial t} &= -\chi_1 \left[ \delta_1 q^2 + \beta_1 + \beta_2 \varphi_1 + \beta_3 \varphi_1^2 + \beta_4 \varphi_1^3 \right. \\ &\quad \left. - 2\beta_3 \frac{\partial^2 \varphi_1}{\partial z^2} + \delta_3 \varphi_2 \right], \\ \frac{\partial \varphi_2}{\partial t} &= -\chi_2 \left[ \delta_2 q^2 + \omega_2 \varphi_2 + M(N)^2 \omega_3 \varphi_2^2 + \omega_4 \varphi_2^3 \right. \\ &\quad \left. - 2M(N)^2 \omega_3 \frac{\partial^2 \varphi_2}{\partial z^2} + \delta_3 \varphi_1 \right]. \end{aligned} \right. \quad (4)$$

In the system of equations (4) time  $t$  is clearly not included, therefore it is an autonomous system of equations. Such equations have multiple solutions. To facilitate their search, self-similar substitutions are used, in which independent variables are associated in a certain way. In our case it is convenient to use the self-similar substitutions of a „running wave“ type expressed as

$$u = z - ct, \quad (5)$$

where  $c$  — kink propagation velocity. As a result, the original system is transformed into a system of ordinary differential equations and the resulting solution will be stationary relative to the new coordinate system.

After substituting (5) in (4) we will obtain

$$\left\{ \begin{aligned} 2\chi_x \gamma_2 M(N)^s \frac{d^2 q_x}{du^2} - 2\chi_x \gamma_1 M(N)^r \frac{dq_y}{du} + c \frac{dq_x}{du} \\ = \chi_x q_x (-\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta_1 \varphi_1 + 2\delta_2 \varphi_2), \\ 2\chi_y \gamma_2 M(N)^s \frac{d^2 q_y}{du^2} + 2\chi_y \gamma_1 M(N)^r \frac{dq_x}{du} + c \frac{dq_y}{du} \\ = \chi_y q_y (-\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta_1 \varphi_1 + 2\delta_2 \varphi_2), \\ c \frac{d\varphi_1}{du} + 2\chi_1 \beta_5 \frac{d^2 \varphi_1}{du^2} = \chi_1 (\delta_1 q^2 + \beta_1 + \beta_2 \varphi_1 \\ + \beta_3 \varphi_1^2 + \beta_4 \varphi_1^3 + \delta_3 \varphi_2), \\ c \frac{d\varphi_2}{du} + 2\chi_2 M(N)^2 \omega_5 \frac{d^2 \varphi_2}{du^2} = \chi_2 (\delta_2 q^2 + \omega_2 \varphi_2 \\ + M(N)^2 \omega_3 \varphi_2^2 + \omega_4 \varphi_2^3 + \delta_3 \varphi_1). \end{aligned} \right. \quad (6)$$

In case of  $\gamma_2 = 0$ ,  $\beta_5 = 0$ ,  $\omega_5 = 0$  the system (6) represents an ordinary first order differential equations system. In the theory of these equations, it is proved that

all integral curves converge to a stationary point, which is defined as the intersection point of the isoclines of horizontal and vertical derivatives (principal or zero isoclines). An isocline, by definition, is the geometric location of points where tangents to integral curves have the same direction. There is no isocline of vertical derivatives in autonomous equations. Therefore, the horizontal isocline is an asymptote for integral curves, and the steady state experimentally detected in [1,3,5,25] is mathematically unattainable in a finite period of time. When the second derivatives are included in the system (6) it results in the rise of damped oscillatory processes with the growth of variable  $u$ .

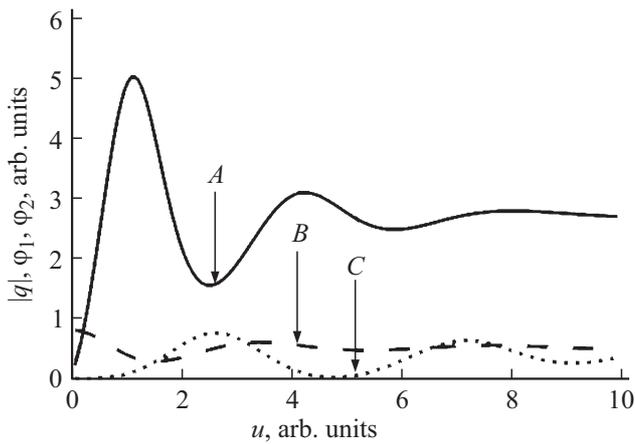
Since it is difficult to find a solution to the system (6) in an analytical form, the mathematical package MatLab was used for numerical analysis. Since the phenomenological parameters specifically for the two-component copper solutions have not been determined, their values were selected from the condition of the solution existence. In the suggested scheme of experiment [1,3,5,25] prior to application of SPTD the sample was annealed. As a result of this effect, the size of the lattice cell also changed. When SPTD was applied, the observed values, regardless of the annealing temperature, asymptotically converged to certain values characteristic of the stationary state. In this paper, a change in the size of a lattice cell describes a structural OP. It is evident that its value depends on the annealing temperature. In this regard, the initial conditions (IC) for the structural OP when solving the system (6) were found complying with the findings from [1,3,5,25]. For the density of screw dislocations, due to their arising only when SPTD was applied, the ICs were taken zero. The initial conditions for the density of the near-band-edge dislocations were determined from the equation of equilibrium in the absence of SPTD.

$$\beta_1 + \beta_2 \varphi_1 + \beta_3 \varphi_1^2 + \beta_4 \varphi_1^3 + \delta_1 q_0^2 = 0, \quad (7)$$

where  $q_0$  — initial condition for the structural OP.

### 3. Discussion of results

The numerical analysis results are presented in Figure 1. The kink motion in the real coordinate system is carried out from the right to the left, i.e., after its passage, the system enters an equilibrium state. The oscillatory nature of this transition, similar to a sequence of solitons, is due to the inertia of the system. These kinks were observed during the wave passage in plasma and are called collisionless. When plotting the graph in Figure 1, the initial conditions for the structural OP were chosen less than its value in the stationary state. However, if the annealing temperature is such that the value of the structural parameter is greater than the stationary one before applying SPTD, then the switching wave will also have an oscillating character with attenuation with the oscillation phase shifted by 180° relative to that shown in Figure 1, but in all cases, the asymptotic behavior will be the same, indicating



**Figure 1.** Configuration of kink (A), densities of the near-band-edge (B) and screw (C) dislocations.

a transition to a stationary state. Figure 1 shows that the frequency of the oscillatory process is not stable. The larger the amplitude, the shorter the oscillation period. Due to the interaction between different OPs, the change in dislocation characteristics also has an oscillatory character with attenuation. Each of these curves approaches the corresponding asymptote. As can be seen from the graph in Figure 1, the extremes of the curves do not coincide at the initial stage. This misalignment is apparently related to the inertia of establishing an equilibrium between the subsystems.

Let us consider the dynamics of dislocation densities as functions of deformation and time. In the hardening and dynamic recovery theory in its atomic dislocation formulation [26,27] it is assumed that the change in dislocation density with increasing degree of deformation  $dq$  for „time“  $du$  is expressed as

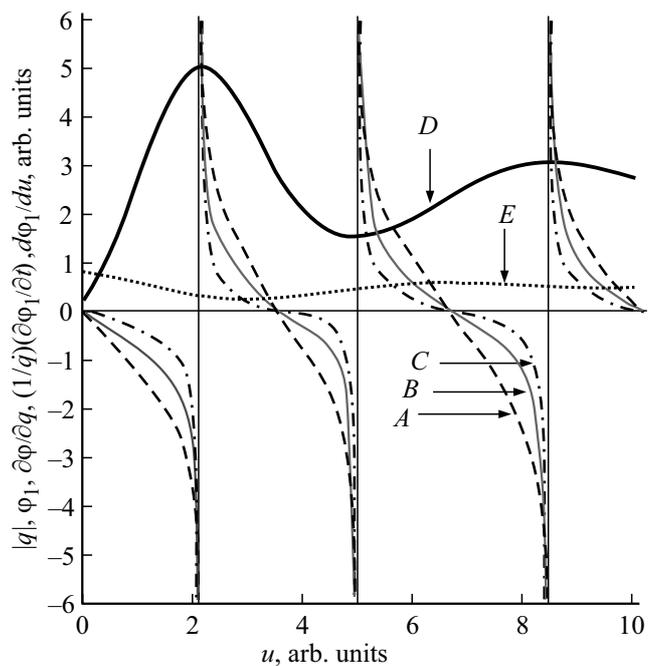
$$d\varphi_i = \frac{\partial \varphi_i}{\partial q} dq + \frac{\partial \varphi_i}{\partial u} du, \tag{8}$$

where  $\partial \varphi_i / \partial q$  — the intensity of dislocation multiplication during deformation,  $\partial \varphi_i / \partial u$  — the intensity of changes in dislocation density due to their generation and annihilation caused by irreversible internal processes, recorded in a self-similar variable. It should be noted, that real velocity is found as  $\partial \varphi_i / \partial t$ , where  $t$  — time, and the signs of these definitions are opposite because of the ratio (5). Then, the total rate of change of densities as functions of deformation is expressed as

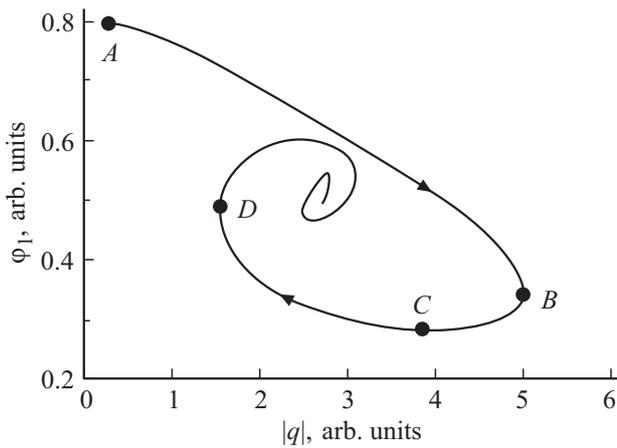
$$\frac{d\varphi_i}{dq} = \frac{\partial \varphi_i}{\partial q} + \frac{\partial \varphi_i}{\partial u} \left( \frac{\partial q}{\partial u} \right)^{-1}. \tag{9}$$

Figure 2 shows the graphs of the first (C) and second (B) terms of the right part of the ratio (9), curve (A) — their sum. As follows from (9), there is a singularity (discontinuity of the second kind) of each term and their sums at the extremum points of the kink dependence on

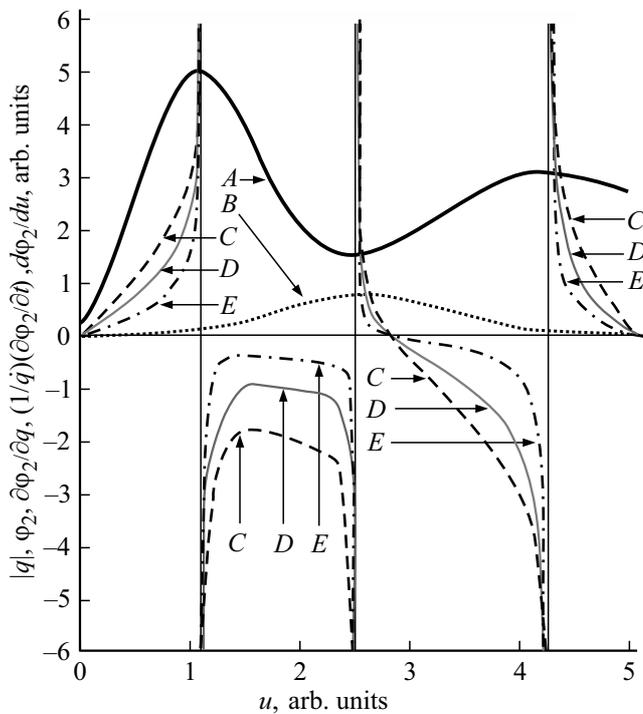
the self-similar variable. Such a singularity means, as shown in Figure 3, a change in the sign of the direction of motion in coordinates  $\varphi-q$ . Vanishing derivatives in Figure 2 correspond to the extremes of the dependence  $\varphi(q)$ . As a result, a structure converging to a certain special point is formed, resembling a logarithmic spiral in shape (Figure 3). The uniqueness of this point (stable focus) is due to the transition of the system to a stationary state. From here it follows that all curves  $\varphi_1(q)$  irrespective of the annealing temperature (initial state) will converge to one point. Let's consider the first interval from zero to the point of the first kink maximum (Figure 2). All the terms of the expression (9) are negative. Consequently, in this interval, the rate of dislocation creations also goes down and, due to the negativity of the second term (9), the rate of annihilation rises, and this process is dominant due to the higher magnitude modulo of the corresponding derivative. As a result the density of dislocations goes down (part of the curve AB, Figure 3). After passing the break point, all derivatives change sign. Moreover, the magnitude of the kink ( $|q|$ ) drops down, which means that  $\varphi-q$  in plane moves backwards (section BD). This interval can be divided in two parts. First part — from the breaking point to the derivatives zero point which stands for motion from point B in Figure 3 to point C. Second part — from zero point to the derivatives breaking point under higher value of variable  $u$  (from point C to point D in Figure 3). In the first interval, all derivatives are positive, but their magnitudes decrease. Consequently, the part of the dislocation density caused by the change in deformation tends to decrease during motion  $B \rightarrow C$ . At the same time, there is a process of



**Figure 2.** Dependences of the near-band-edge dislocations' creation and annihilation rates and their sum. See explanation in the text.



**Figure 3.** Dislocations densities  $\phi_1$  versus deformation during application of SPTD.

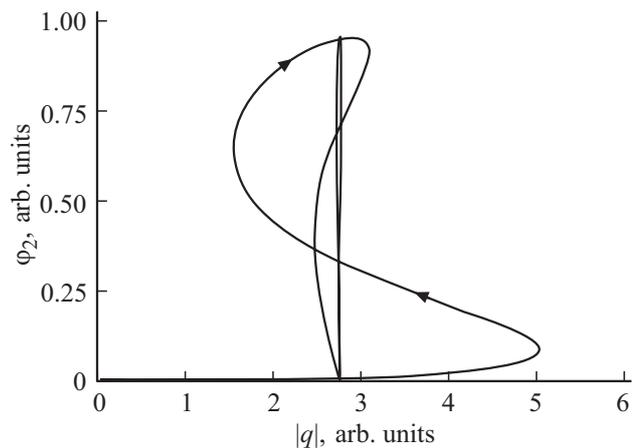


**Figure 4.** Dependences of the screw dislocations' creation and annihilation rates and their sum. See explanation in the text.

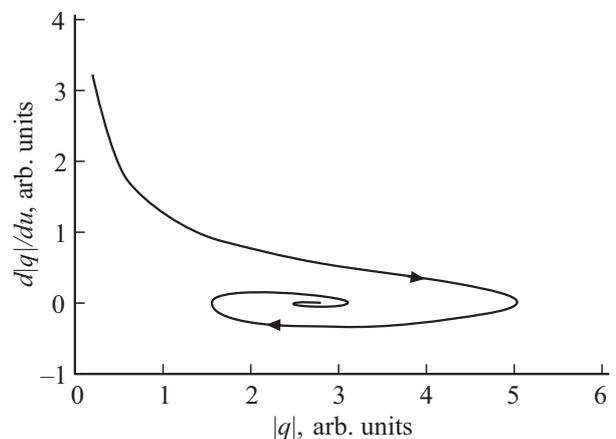
strong creation inhibition due to internal processes, and the total dislocation density goes down (see Figure 3, lower branch BC). In the second interval, all derivatives of the self-similar variable are negative, but when moving in the opposite direction, they decrease in absolute value. Consequently, the processes responsible for the increase in dislocation density prevail (Figure 3, section CD). Since the peak-to-peak swing of the kink subsides in subsequent intervals, the spiral in Figure 3 twists into a point.

It is of interest to conduct a similar analysis for the spiral dislocation that occurs when SPTD is applied. As can be

seen from Figure 1, the peak-to-peak swing and appropriate instantaneous densities frequencies  $\phi_1$  and  $\phi_2$  do not coincide. In this regard, the behavior of the corresponding derivatives differs significantly. Figure 4 shows the results of calculations. Curves A and B — curves of kinks and screw dislocation density, D, E and C — rates of annihilation, creation and their sum respectively. This difference is due to the fact that the synchronization of the vibrations of the screw and structural OP is achieved at high values of the variable  $u$ . Because of this, the sign of all derivatives in the intervals where there is no synchronization does not change. In particular, in the first interval  $0 < u < 1$  all derivatives are positive, and in the second  $1 < u < 2.5$  (the first interval between the singularities) — they are negative (Figure 4). Also, at both intervals, the dependencies of both OP change monotonously. In the third interval  $2.5 < u < 4.2$  (the second interval between the singularities), the behavior of the dependence  $\phi_2(q)$  changes significantly, and it becomes non-monotonic. Further, the relationship of behavior of the dependencies under consideration becomes similar to those shown in Figure 2. However, it should be emphasized, that fluctuations in the density of the screw dislocation are



**Figure 5.** Dislocations densities  $\phi_2$  versus deformation during application of SPTD.



**Figure 6.** Phase portrait of a structural OP when SPTD is applied.

characterized by a small decrement. All this leads to the fact that the phase trajectory resembles a figure of eight (Figure 5). As the variable  $u$  grows, the figure-of-eight loops narrow, and as  $u$  rises, it degenerates into a straight line segment with decreasing length and collapsing into a point at infinity (stable focus).

Figure 6 illustrates the phase portrait of a structural OP. Obviously, the singular point, which is a stationary state, is a stable focus, and the phase trajectory is approximately a logarithmic spiral. This behavior of the trajectory describes the instability of the system state in the transition layer, which is confirmed by the oscillating behavior of the structural OP shown in Figure 1.

Phase portraits of dislocation densities behave in almost the same way. The difference between them is the speed of twisting and the shape of the loops when moving towards a stable focus.

## 4. Conclusions

Theoretically, it is predicted that the boundary of transition (kink) to the stationary state when SPTD is applied is not a step and has a finite width in space, within which the transition is an oscillating process with attenuation. Due to the oscillatory processes in the transition region, singularities of dislocations creation and annihilation rates occur as functions of deformation.

## Funding

The work was supported by the Ministry of Education and Science of Russia on the topic „Formation of the structure and properties of promising multifunctional materials“ (FREZ-2023-0001) for FBGNU „Donetsk physical-technical institute named after A.A. Galkin“.

## Conflict of interest

The authors declare that they have no conflict of interest.

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*Translated by T.Zorina*