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Establishing the stationary state during severe plastic deformation by twisting in two-component crystals

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Received December 24, 2021
Revised December 24, 2021
Accepted December 27, 2021

The propagation of a switching wave (kink) in two-component crystals during plastic torsion strain has been considered. The phenomenological Landau theory with consideration of Lifshitz invariants was used. A numerical simulation of the shape of the kink that occurs under various temperatures has been performed.

Keywords: kink, order parameter, torsion, potential, two-component crystal.

DOI: 10.21883/PSS.2022.04.53501.263

1. Introduction

A current issue at present is the behavior of materials under severe plastic torsional deformation (SPTD). As shown in [1,2], application of SPTD may change the phase composition of two-component materials such as Cu−Ag, Cu−Sn, Cu−Co. Thereat, the non-destructive process of torsion impact took place. It was found that, if the number of revolutions is large enough, a system always comes to the same stationary state irrespective of the initial state and annealing temperature. The phase boundary of the diagram of dependence of dissolved impurity concentration on annealing temperature T_{ann} shifted and degenerates into a straight vertical line [1]. Concurrently, a change in the lattice parameters occurred simultaneously. Such a behavior of the observed quantities can be explained on the basis of the Landau's phenomenological theory [3,4]. However, these papers did not consider the wave edge shape (kink) arising under SPTD. The present paper is dedicated to studying this issue. Movement of the edge is an autowave process in the kink form and is the simplest topological soliton. A stationary state established after the edge passes through the entire crystal. Autowaves arise in various physical, chemical and biological media. Their examples can be concentration waves in the Belousov−Zhabotinsky reaction [5], chemical signaling waves in colonies of certain microorganisms [6], waves in the interstellar gas which lead to the formation of spiral galaxies [7]. An important example of active media is many biological tissues. Thus, propagation of a neural impulse [8] and excitation in the cardiac muscle have the autowave nature [9]. Self-similar solutions of a differential equation in physical systems correspond to motion of the phase interface under first- or second-order phase transitions [10,11], and describe flame propagation [12]. The above-mentioned papers describe the found analytical approximate solutions. Paper [13] describes an attempt at a numerical consideration of this issue, which provides a more accurate solution. In the present paper the ideas elaborated in [3,4,13] are applied to two-component crystals.

2. Theory

Let a two-component crystal with one fastened end be exposed to SPTD in the phase diagram region where the impurity is completely dissolved. In the present paper we will consider the behavior of the edge (kink) of an arising traveling wave. In this case a virtual crystal approximation can be used. If it is used, all the crystal characteristics are assumed to be averaged and we can introduce a unified order parameter (OP) to describe unit cell deformation. Let us use the Landau's phenomenological theory to establish the kink shape.

As shown in [10,11], kink dynamics can be conveniently considered using a differential equation of the Landau−Khalatnikov type [14]:

$$\frac{\partial q_i}{\partial t} = -\gamma_{ii}\frac{\delta\widetilde{\Phi}}{\delta q_i}; \quad (i = x, y), \tag{1}$$

where $\widetilde{\Phi}$ is the composed function of free energy,

$$\frac{\delta\widetilde{\Phi}}{\delta q_i} = \sum_k (-1)^k \frac{d^k}{dz^k}\frac{\partial\Phi}{\partial\left(\frac{\partial^k q_i}{\partial z^k}\right)}$$

— functional derivative, t — time, $\gamma_{ii}(i = x, y)$ — components of the parameter that characterizes the rate of

system relaxation to an equilibrium position. We will subsequently assume that these components are constant and will neglect the off-diagonal components for simplicity. The Landau–Khalatnikov equation is an equation in partial derivatives in relation to time (the left member) and spatial variables (the right member) and describes the process of relaxation from one state to another. The equation was created based on the fact that a physical system reaches a stationary state at $t \to \infty$. Depending on the right member, such a transition can be smooth, abrupt or via several intermediate states. Transition kind is affected by dispersion, dissipation, relaxation rate and other factors. The Landau−Khalatnikov equation allows many solutions dependent on kind of non-equilibrium thermodynamic potential and magnitude of its parameters. This equation describes the relaxation processes, both in perfect crystals and in defective crystals. Various deviations from the perfect structure in the non-equilibrium thermodynamic potential NTDP are determined using derivatives of different orders from the corresponding OPs according to spatial variables. In particular, long-period spiral structures in crystals without an inversion center can be described using Lifshitz invariants. If the crystal has an inversion center, squares of the first and second derivatives must be introduced in the NTDP. In the latter case, the system of equations (2) becomes a fourth-order system in relation to space derivatives, which requires a large number of initial (boundary) conditions and the solution is complicated. Therefore, we will restrict ourselves to crystals without an inversion center.

Density of a NTDP-system, exposed to SPTD with moment M along the OZ axis, is as follows [3,4,13,15]:

$$\widetilde{\Phi} = \frac{\alpha_1}{2} q^2(N) + \frac{\alpha_2}{4} q^4(N) + \frac{\alpha_3}{6} q^6(N) + \gamma_1 M^r \times \left(q_x \frac{\partial q_y}{\partial z} - q_y \frac{\partial q_x}{\partial z} \right) + \gamma_2 M^s \left(\left(\frac{\partial q_x}{\partial z} \right)^2 + \left(\frac{\partial q_y}{\partial z} \right)^2 \right) + \beta_1 \varphi + \frac{\beta_2}{2} \varphi^2 + \frac{\beta_3}{2} \varphi^3 + \delta q^2 \varphi, \quad (2)$$

where $\gamma_i (i = 1, 2)$, α_i, β_i $(i = 1{-}3)$, δ — phenomenological constants, q — vector structural OP with components q_x and q_y, defined as a linear combination of shifts of unit cell ions as a result of a phase transition, φ — defect density. The component q_z is ignored, since the torque moment is along the OZ axis. In fact, the present paper considers the possibility of origination of transverse waves only. Torque moment M is an axial vector. Therefore, the powers r and s in (1) must be even in crystals without an inversion center. As demonstrated in [13], $r = 6$, $s = 2$. The term accountable for elastic interaction is not written out in potential (1). The procedure for its exclusion is given in [16]. It must be noted that the Lifshitz invariants, which describe the deformation arising under SPTD, are absent in crystals with an inversion center, since the arising axial symmetry does not remove the inversion. Therefore, crystals without an inversion center are considered in the present paper. Substituting (2) in (1), we obtain

$$\begin{cases} \dfrac{\partial q_x}{\partial t} = -\gamma_{xx} \left[q_x(\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta\varphi) + 2\gamma_1 M^r \dfrac{\partial q_y}{\partial z} - 2\gamma_2 M^s \dfrac{\partial^2 q_x}{\partial z^2} \right] \\ \dfrac{\partial q_y}{\partial t} = -\gamma_{yy} \left[q_y(\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta\varphi) - 2\gamma_1 M^r \dfrac{\partial q_x}{\partial z} - 2\gamma_2 M^s \dfrac{\partial^2 q_y}{\partial z^2} \right] \end{cases}. \quad (3)$$

As shown in [3,4], magnitude of defect density φ depends on annealing temperature T_{ann}. Since the corresponding law is unknown, the desired dependence was selected by a best fit of the theoretical and experimental data. Since the dependence is weak, we neglect it. The obtained system of equations is autonomous and can be considerably simplified by changing over to a self-simulated variable

$$u = z - ct, \quad (4)$$

where c is the phase velocity of wave propagation. Mathematically this conversion means a changeover to a moving coordinate system where a wave is immobile, and a distribution of characteristics at different time moments is obtained by shifting. It is clear that the class of system solutions narrows and it is simpler to find a solution. As a result, a system of ordinary differential equations is obtained

$$\begin{cases} 2\gamma_{xx}\gamma_2 M^s \dfrac{d^2 q_x}{du^2} - 2\gamma_{xx}\gamma_1 M^r \dfrac{dq_y}{du} + c \dfrac{dq_x}{du} = \gamma_{xx} q_x(\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta\varphi) \\ 2\gamma_{yy}\gamma_2 M^s \dfrac{d^2 q_y}{du^2} + 2\gamma_{yy}\gamma_1 M^r \dfrac{dq_x}{du} + c \dfrac{dq_y}{du} = \gamma_{yy} q_y(\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta\varphi) \end{cases}. \quad (5)$$

In order to solve this system, we must assign four conditions which can be $q_x(-\infty)$, $q_y(-\infty)$, $q_x(+\infty)$, $q_y(+\infty)$. Since the system is in an equilibrium state at $t = 0$ and a random value of $z\,(u = z)$ (there is no SPTD.), all the derivatives are zero. Consequently, quantity $q(+\infty)$ is determined from a system of algebraic equations

$$\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\delta\varphi = 0. \quad (6)$$

Considering the uncertainty, we adopt $q_x(+\infty) = q_y(+\infty) = \frac{q(+\infty)}{\sqrt{2}}$.

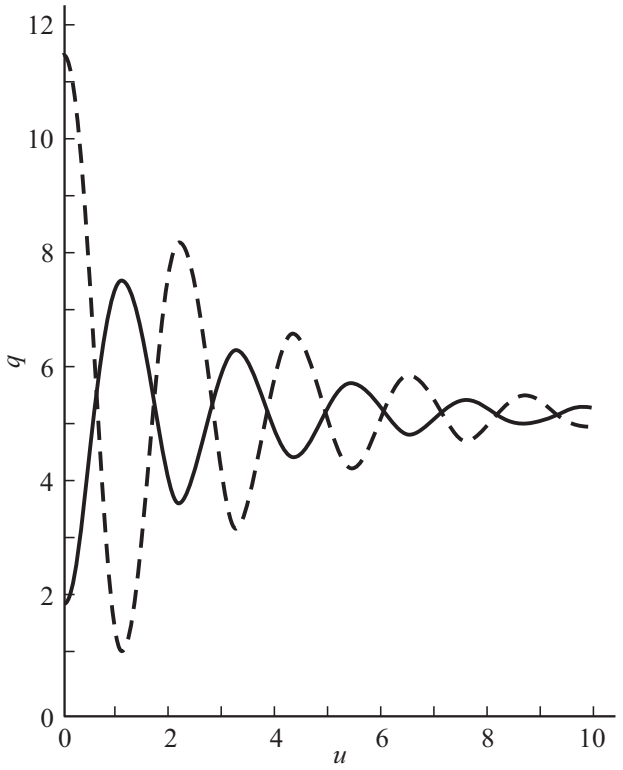

Figure 1. Qualitative kink shape at a low velocity. Arbitrary units of measurements are adopted along the axes.

It was shown in [3,4] that the magnitudes of coefficients $\alpha_i (i = 1-3)$ depend on annealing temperature and, therefore, stationary states will slightly differ from each other. However, we neglect this insignificant difference in the present paper for simplicity. At $t = +\infty$ $(u = -\infty)$, the system is also in an equilibrium state, and under SPTD it has a crystalline spiral structure described by relations $q_x = q(-\infty) \cdot \cos(k \cdot z)$, $q_y = q(-\infty) \cdot \sin(k \cdot z)$. Here the OP modulus is a constant quantity. To find the next pair of boundary conditions, we must substitute these relations in (3) taking into account the fact that all time derivatives are zero. Simple conversions yield a biquadratic algebraic equation solved as follows [3]:

$$q^2(-\infty) = \frac{-\alpha_2 + \sqrt{\alpha_2^2 + 4\alpha_3 \left(\alpha_1 - 2\delta\varphi + \frac{\gamma_1^2 M^{2r-s}}{2\gamma_2} \right)}}{2\alpha_3}. \tag{7}$$

Here we also adopt $q_x(-\infty) = q_y(-\infty) = \frac{q(-\infty)}{\sqrt{2}}$. As shown in [1–4], a critical annealing temperature $T_{kr\,ann}$ is observed in two-component systems such as Cu–A (A = Ag, Sn, Co); system's behavior drastically changes after a transition through this temperature. At $T_{ann} < T_{kr\,ann}$, the function $q(N)$, where N — number of revolutions — is increasing and convex, at $T_{ann} > T_{kr\,ann}$ the desired dependence is decreasing and concave. This behavior is explained by the divergence and a change of the sign of coefficient γ_2 in the vicinity of point $T_{ann} < T_{kr\,ann}$ [3,4]. This peculiarity affects the kink shape as well.

Fig. 1 shows the established propagation mode for relatively long times after SPTD impact and presents the dependence $q(u)$ for the case $T_{ann} < T_{kr\,ann}$ (solid curve) and $T_{ann} > T_{kr\,ann}$ (dashed curve). In both cases there is an oscillatory process upon a transition from one state to another. This peculiarity of the kink leading edge depends on its velocity and relaxation coefficient magnitude. An increase of propagation speed leads to an increase of oscillatory process decay, i.e. the amplitude and number of oscillations till transition to an equilibrium state decrease. The kink shape in the high speed limit becomes monotonic (decreasing or increasing). When the relaxation coefficient increases, oscillation amplitudes of the leading edge and their number increase. A decrease of γ acts similarly to an increase of unperturbed velocity.

A decrease of the value of coefficient γ_2 leads to an increase of the damped oscillations frequency and does not affect their amplitude. Thereat, a transition to the final stationary state is faster (Fig. 2). It should be noted that similar oscillating tails of solitons were predicted in [17].

Behavior of the leading edge can be affected by dispersion, magnitude of which is defined to be constant γ_1. Let us assume that a weak dispersion is due to a change of the OP magnitude. Then γ_1 can be expanded into a series according of OP powers. Let us consider two cases.

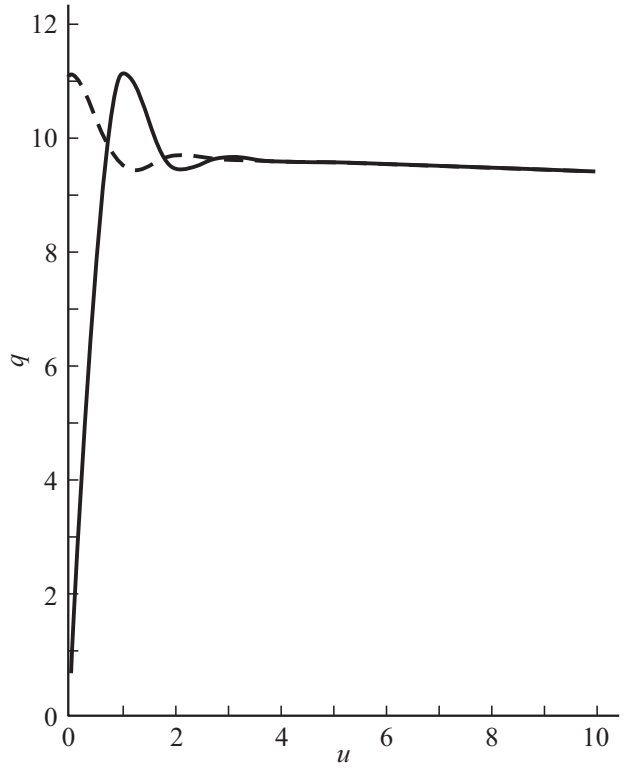

Figure 2. Qualitative kink shape at a high velocity. The solid line shows $T_{ann} < T_{kr\,ann}$. The dashed line shows $T_{ann} > T_{kr\,ann}$. Arbitrary units of measurements are adopted along the axes.

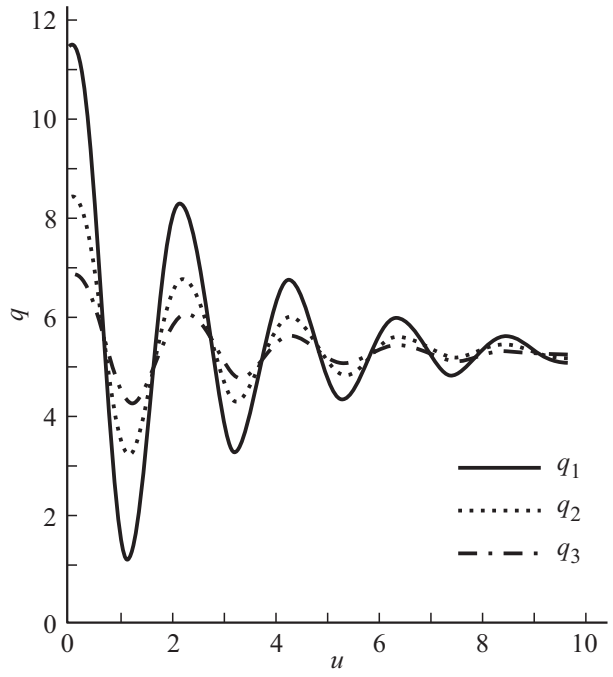

Figure 3. Comparison of qualitative shapes of the kink with quadratic (dashed line) and linear (dash-and-dot line) dependences of dispersion on OP. The solid line means no dispersion. Arbitrary units of measurements are adopted along the axes.

1. Quadratic dependence: $\gamma_1 = \gamma_{10} + \gamma_{11}\left(q - q(+\infty)\right)^2$. The corresponding system of auto-wave equation is as follows

$$\begin{cases} 2\gamma_{xx}\gamma_2 M^s \dfrac{d^2 q_{2x}}{du^2} - 2\gamma_{xx}\Big(\gamma_{10} + \gamma_{11}\left(q_2 - q_2(+\infty)\right)^2 \\ \quad + 2\gamma_{11}\left(q_{2x} - q_{2x}(+\infty)\right)\Big) M^r \dfrac{dq_{2y}}{du} + \Big(c + 2\gamma_{xx}\gamma_{11}M^s \\ \quad \times \left(q_{2x} - q_{2x}(+\infty)\right)\left(q_{2y} - q_{2y}(+\infty)\right)\Big) \dfrac{dq_{2x}}{du} \\ = \gamma_{xx} q_{2x}(\alpha_1 + \alpha_2 q_2^2 + \alpha_3 q_2^4 + 2\delta\varphi) \\ 2\gamma_{yy}\gamma_2 M^s \dfrac{d^2 q_{2y}}{du^2} + 2\gamma_{yy}\Big(\gamma_{10} + \gamma_{11}\left(q_2 - q_2(+\infty)\right)^2 \\ \quad + 2\gamma_{11}\left(q_{2y} - q_{2y}(+\infty)\right)\Big) M^r \dfrac{dq_{2x}}{du} + \Big(c + 2\gamma_{yy}\gamma_{11}M^s \\ \quad \times \left(q_{2x} - q_{2x}(+\infty)\right)\left(q_{2y} - q_{2y}(+\infty)\right)\Big) \dfrac{dq_{2y}}{du} \\ = \gamma_{yy} q_{2y}(\alpha_1 + \alpha_2 q_2^2 + \alpha_3 q_2^4 + 2\delta\varphi) \end{cases} \tag{8}$$

The plot of a numerical solution for this system with account of the initial conditions (6) and (7) is shown in Fig. 3 by a dashed line. The solid line shows the shape of kink ($q_1(u) = q(u)$) at $\gamma_1 = \text{const}$. A considerable decrease of the leading edge maxima can be seen. This conclusion is confirmed by the plots of the corresponding OP shift velocities shown in Fig. 4. It must be noted that qualitative behavior of OPs in the right part of the kink's leading edge is virtually the same in both cases.

2. Linear dependence: $\gamma_1 = \gamma_{10} + \gamma_{11}\left(q - q(+\infty)\right)$. System of equations

$$\begin{cases} 2\gamma_{xx}\gamma_2 M^s \dfrac{d^2 q_{3x}}{du^2} - 2\gamma_{xx}\Big(\gamma_{10} + \gamma_{11}\left(q_3 - q_3(+\infty)\right) \\ \quad + \gamma_{11}\dfrac{\left(q_{3x} - q_{3x}(+\infty)\right)^2}{2\left(q_3 - q_3(+\infty)\right)}\Big) M^r \dfrac{dq_{3y}}{du} + \Big(c + \gamma_{xx}\gamma_{11}M^s \\ \quad \times \dfrac{\left(q_{3x} - q_{3x}(+\infty)\right)\left(q_{3y} - q_{3y}(+\infty)\right)}{q_3 - q_3(+\infty)}\Big) \dfrac{dq_{3x}}{du} \\ = \gamma_{xx} q_{3x}(\alpha_1 + \alpha_2 q_3^2 + \alpha_3 q_3^4 + 2\delta\varphi) \\ 2\gamma_{yy}\gamma_2 M^s \dfrac{d^2 q_{3y}}{du^2} + 2\gamma_{yy}\Big(\gamma_{10} + \gamma_{11}\left(q_3 - q_3(+\infty)\right) \\ \quad + \gamma_{11}\dfrac{\left(q_{3y} - q_{3y}(+\infty)\right)}{2\left(q_3 - q_3(+\infty)\right)}\Big) M^r \dfrac{dq_{3x}}{du} + \Big(c + \gamma_{yy}\gamma_{11}M^s \\ \quad \times \dfrac{\left(q_{3x} - q_{3x}(+\infty)\right)\left(q_{3y} - q_{3y}(+\infty)\right)}{q_3 - q_3(+\infty)}\Big) \dfrac{dq_{3y}}{du} \\ = \gamma_{yy} q_{3y}(\alpha_1 + \alpha_2 q_3^2 + \alpha_3 q_3^4 + 2\delta\varphi) \end{cases} \tag{9}$$

The dash-and-dot lines in Fig. 3, 4 show the numerically found dependences of kink front ($q_3(u)$) and the corresponding derivative. The OP oscillation amplitudes decrease in the right half of the leading edge, which leads to a smaller

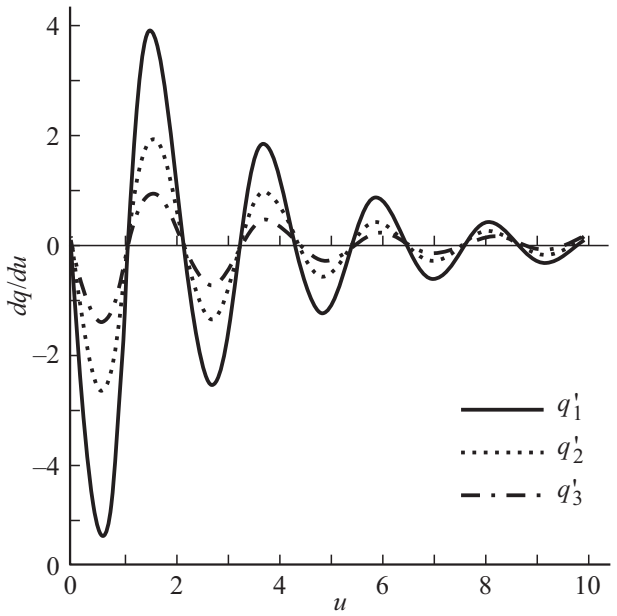

Figure 4. Qualitative shape of OP derivatives with quadratic (dashed line) and linear (dash-and-dot line) dependences of dispersion. The solid line means no dispersion. Arbitrary units of measurements are adopted along the axes.

OP value for the final stationary state. The derivatives in the right part of the leading edge also have an identical shape.

It must be noted that derivatives at point $u = 0$ are zero in all cases, i.e. there is a minimum of the oscillatory process in relation to the final state. This point is stable since the first OP derivative is zero, and the energy minimum is ensured. The situation is similar in the task of thermal edge propagation [17]. We showed that a local maximum at the initial point is possible only in plane symmetry systems, which is true in our problem. If symmetry is axial or ball, the first-order derivative at point $u = 0$ is non-zero.

3. Conclusion

1. It is shown that oscillations with an increasing amplitude occur in the leading edge at a low velocity of kink propagation.

2. If kink propagation velocity is high, the leading edge is a monotonic curve.

3. Dispersion significantly affects the kink shape. Oscillation amplitudes decrease in the case of linear and quadratic dispersions, but the frequency pattern does not change.

Conflict of interest

The authors declare that they have no conflict of interest.

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