

A Frank-Read Source Model

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Abstract

The temporal dynamics of the edge dislocation (ED) was studied in this work using the inhomogeneous dissipative sine-Gordon (SG) equation. The consideration was carried out for the force action levels both less and more critical. By SG equation numerical calculations it is shown that at the external force value below a critical one the ED takes a shape close to a semicircle. This shape was used as an initial condition for describing the ED temporal dynamics in the FR source operating mode. A particular solution of the SG equation is proposed that describes the temporal dynamics of half the ED in the FR mode, which rests on a stopper at the origin. It is shown that the proposed particular solution corresponds to the left Archimedes spiral displaced at $\pi/2$ counterclockwise relative to the azimuth angle equal to zero. It is noted that the temporal dynamics of the second half of the ED segment rested on the second stopper is described by the proposed particular solution, when it is mirrored relative to the problem symmetry axis and the center of the spiral is displaced to a point with a zero azimuthal angle and a radius equal to the distance between the stoppers. The axis of symmetry is a straight line that is perpendicular and halves the distance between the stoppers. A graphical description of the ED temporal dynamics was plotted in the Cartesian coordinate system based on the proposed particular solution and its mirror and displaced image. It is shown that the particular solution of the SG equation in the RF source operation mode involves two Archimedes spirals symmetrical relative to the problem symmetry axis with equal radii increasing linearly with time, which rotate: one (the spiral center coincides with the stopper at the origin) counterclockwise, the second (the spiral center coincides with the second stopper) clockwise.

Keywords

Edge Dislocation, Sine-Gordon (SG) Equation, Frank-Read Source, Archimedes Spiral, Temporal Dynamics

1. Introduction

The mechanism of continuous generation of dislocations in the slip plane was first proposed by Frank and Reed [1]. This mechanism is based on consideration of the displacement of the edge dislocation (ED) fixed at both ends at points O and O' under the external force action. Two immobile dislocations CO and DO' not lying in the slip plane, atoms of a dissolved substance or particles of precipitates can be as fixation points of the dislocation. With a gradual increase in the external force action, the shear stress can reach a critical value at which the dislocation begins to move in the direction of the force.

We shall call the region into which the dislocation moves as frontal. The required shear stress τ_0 is determined by the following expression $\tau_0 = bG/L$: where G —the crystal shear modulus, L —the ED length and b —the length of the Burgers vector. For a dislocation line in the form of a semicircle the applied stress is maximal, but after passing through this state the dislocation becomes unstable and continuously expands [2]. At any point of the dislocation line acts the same constant stress $\sigma_n = \tau b$, so its movement velocity at each point is also the same. Therefore, the dislocation line near the fixing points is twisted into two spirals rotating in opposite directions. Dislocation loops are formed at a stage when in the backside of the dislocation (the side opposite the frontal) the rotated spirals will touch one another. At the contact point the dislocations annihilate due to the fact that the Burgers vector of each of them has an equal length but opposite direction. As a result a closed dislocation loop is formed, which continues to expand under the action of the applied stress. The remains spirals located between the contact point and the fixing points form again the initial ED under the action of the applied stress. When keeping the action of the external stress the above cycle repeats, the described process of the formation of dislocation loops is usually called the Frank—Reed source (FR).

Thus, multiply repetition of the cycle described above generates an endless series of loops. This process will continue until the back stresses arising at the dislocation interaction and counteracting the applied stresses balance the action of the external stress.

Figure 1 shows the successive stages of the FR source action, which end with formation of a dislocation loop 4 from the ED. At that, a constant stress σ_n directed along the normal acts on the dislocation line at each of its points (vectors of the stress σ_n are not shown in the figure).

Visual representation of the FR source operation described in **Figure 1** is based on quasistatic models based on the description of stress fields arising around the edge dislocation [3] [4] [5] [6] [7]. Using such models makes it possible to determine some static parameters of crystalline materials. However, these models are not applicable to describe the ED strain development in time.

Let us briefly discuss the results of previous studies of the ED deformation in time in the FR source mode.

Until the present time, no analytical description of such processes has existed.

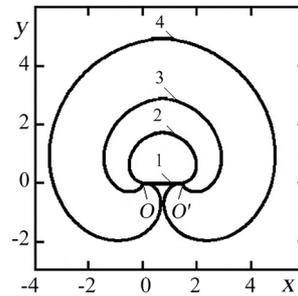


Figure 1. Stages (2, 3, 4) of formation of the dislocation loop from the ED (1). The axis x is directed along the initial position of the ED, the axis y determines the deviation of the ED from the equilibrium position (x and y are measured in units of the lattice spacing b).

Therefore the answer to this question was obtained by numerical simulation methods in a number of works. Numerical analysis of the ED deformation was carried out for partial differential equations of hyperbolic [8]-[14] or parabolic [15] [16] [17] type.

However, the drawback of numerical calculations is that they do not determine the analytical dependence of the ED deformation on time and its characteristic parameters, which complicates the understanding of the process physics.

By numerical study of partial differential equations of a hyperbolic type the following results were obtained.

In [14] within the framework of the dislocation string model (the Frenkel-Kontorova model [8]), the ED nonlinear dynamics under the effect of the external harmonic force was studied by numerical methods.

The calculations have shown that at sufficiently high amplitude of the external harmonic force the oscillation amplitude of the dislocation string can be comparable with the lattice spacing. Under such conditions, the dislocation movement is possible both in the direction of the climb force and in the opposite direction. The resonant nature of the increase in the average kinetic energy of the string depending on the frequency of the external harmonic force was shown. The process considered in the work is indicative by using a partial differential equation of a hyperbolic type in the case of action of a time-periodic force. This example does not lead to the task of studying the FR source generation, but describes the generation of multi-soliton solutions on ED.

In [18] it is shown that in a constant field of stresses the ED can form FR sources. At that, FR source operation is accompanied by an acoustic emission (AE).

In the paper [19] a plane dislocation loop has been considered, which, as a result of the FR source operation, emits AE in a medium with a sufficiently large dislocation friction coefficient. It is shown that in the dipole approximation the loop expands under the action of a uniform external stress σ_0 up to the radius R_0 and then it instantly stops at stoppers. The similar model of dislocation cluster formation is described in [12] and comes to an agreement with the con-

clusion that the loop area at the stage of its leaving the source varies with time according to the quadratic law [18].

However, the above calculations do not specify the temporal dynamics of the loop shape change starting from the moment of its rotation relative to the stoppers. This information is of interest for understanding both the physics of the formation of the first loop and the following loops.

Using partial differential equations of hyperbolic type to describe the ED temporal dynamics [15] [16] [17] changes the physics of the process from wave, when ED segments take part in wave motion, to diffusion, when ED segments displacement is subject to diffusion. In the latter case a numerical analysis of the position of the dislocation curve segment is based on its position obtained in the previous step. Although numerical calculations describe the formation of loops rather well, it is required to use smoothing factors (Gibbs phenomenon [20]) in the calculation algorithm in order to provide calculations for the entire range of physical parameters.

The aim of this work is to obtain, within the framework of the ED string model, an analytical solution for ED temporal dynamics in the field of non-oscillating external stress in the FR source operation mode.

The following steps were taken to solve the task of studying the ED strain in the FR source operating mode:

- 1) The initial equation describing the process of ED shape change in time is selected and the process itself is divided into two stages: the first, when the ED takes a shape close to the semicircle, and the second, corresponding to ED operation in the FR source mode;
- 2) Study of the first stage of the ED temporal dynamics, when the force effect is less than the critical level;
- 3) Study of the ED temporal dynamics in the FR source operation mode.

2. Initial Equation and Two Stages of the Temporal Dynamics of ED

Following the Frenkel-Kontorova model we will consider the edge dislocation of a length L as a string that is located on the axis ox and its ends are fixed at points with coordinates $\{0, L\}$. The string displacements occur in the slip plane xy . In this geometry the displacement of the dislocation segment of the edge dislocation $w(x, t)$ is determined by the well-known inhomogeneous dissipative sine-Gordon equation (SG) [21] [22] [23]:

$$m \frac{\partial^2 w}{\partial t^2} - K_0 \frac{\partial^2 w}{\partial x^2} + b\sigma_p \sin\left(\frac{2\pi w}{a}\right) = bF(t) - \delta' \frac{\partial w}{\partial t}, \quad (1)$$

with boundary conditions at fixation points called stoppers:

$$w(0, t) = w(L, t) = 0, \quad (2)$$

where: $m = \left(\frac{\rho b^2}{4\pi}\right) \ln\left(\frac{L}{b}\right)$ — effective mass of the dislocation length unit; ρ —

crystalline substance density; b —Burgers vector module;

$\delta' = (10^{-5} - 10^{-2}) \text{kg}/(\text{m} \cdot \text{s})$ [13] [24] [25]—dislocation friction coefficient;

$K_0 = G \frac{m}{\rho}$ —dislocation linear tension coefficient; G —crystal shear modulus;

$\sigma_p = (10^{-4} - 10^{-2})G$ —Peierls characteristic stress; $L = (10 - 10^4)b$ —characteristic dislocation length; $F(t)$ —external stress.

The characteristic parameters of a dislocation string can take the following values [26]:

$$m \approx 10^{-16} \text{ kg/m}; \quad G \approx 50 \text{ GPa}; \quad \frac{a}{2} = \frac{b}{3} \approx 10^{-10} \text{ m};$$

$$\sigma_p \cdot 10^3 \approx \sigma_0 \cdot 10^4 \approx G; \quad P \approx (10^{-3} - 10^{-1})G. \quad (3)$$

Equation (1) is also used to describe the nonlinear dynamics of physical systems of various types (dislocations and crowdions in solids, domain boundaries, Josephson contacts, biological molecules, and crystal surfaces) [23].

The first and second terms of the right-hand side of Equation (1) describe the contribution of external stresses and internal dissipation, respectively.

3. The First Stage of the Temporal Dynamics of ED When Taking into Account an External Stress

For the dimensionless displacement value $R = \frac{2\pi w}{a}$ and in dimensionless variables $t = \zeta t_0$, $x = \xi x_0$ Equation (1) and boundary conditions (2) take the form:

$$\frac{\partial^2 R}{\partial \zeta^2} - \frac{\partial^2 R}{\partial \xi^2} + \sin(R) = \Phi(\zeta) - \delta \frac{\partial R}{\partial \zeta}$$

$$R(0, \zeta) = R\left(\frac{L}{x_0}, \zeta\right) = 0 \quad (4)$$

where: a —crystal lattice constant; $t_0^2 = \frac{a \cdot m}{2\pi b \sigma_p}$; $x_0 = s_0 t_0$; $s_0^2 = \frac{K_0}{m}$;

$$\delta = \frac{\delta'}{m} t_0; \quad \Phi(\zeta) = \frac{F(\zeta)}{\sigma_p}.$$

For ED parameters (3) the characteristic time t_0 , distance x_0 , and velocity s_0 have the following order of magnitude: $t_0 \sim 4.6 \times 10^{-12} \text{ s}$; $x_0 \sim 1.3 \times 10^{-8} \text{ m}$; $s_0 \sim 2.9 \times 10^3 \text{ m} \cdot \text{s}^{-1}$.

We consider that the external stress on the right side of Equation (4) is a sufficiently large value, *i.e.* $|\Phi(\zeta)| \geq 1$. The stress action of this magnitude can create conditions under which the ED operates as a FR source.

It is known that after passing the critical level of force action the ED takes a shape close to a semicircle and begins to expand [2]. Therefore, the ED temporal dynamics can be divided conventionally into two stages. At the first stage the ED takes a shape close to a semicircle. At the second stage the ED continuously ex-

pands and begins to operate as the FR source.

To analyze the nature of the ED displacement at the first stage of the external force action the numerical calculations were carried out. These calculations show that at ED displacement amplitudes smaller than the lattice spacing the semicircle formation is observed. **Figure 2** shows the swept ED surface from the view of which it can be concluded that the ED forms a curve close in shape to a semicircle for the following parameters of Equation (4): $\Phi(\zeta) = 0.01 \cdot \zeta$, $\delta = 0.1$.

The analysis of the second stage of the ED temporal dynamics is based on using the ED shape close to semicircle as an initial one.

Let us consider the ED temporal dynamics after passing the critical level of the force action, which describes the FR source operation.

4. ED Temporal Dynamics in FR Source Operation Mode

Let us consider the conditions under which the solution of Equation (4) described the FR source can be realized.

We divide the ED into two symmetric halves relative to the coordinate $\xi_{FR} = L/2x_0$. We will seek a solution of Equation (4) in the half-plane I ($\xi \leq \xi_{FR}$). In the half-plane II ($\xi \geq \xi_{FR}$) the solution will be symmetric relative to $\xi = \xi_{FR}$ and such, that $R_I(\xi_{FR}, \zeta) = R_{II}(\xi_{FR}, \zeta)$,

$R_{II}(\xi, \zeta)|_{\xi_{FR} \leq \xi \leq 2\xi_{FR}} = R_I(\xi_{FR} - \xi, \zeta)|_{0 \leq \xi \leq \xi_{FR}}$, where indices I and II indicate that the solution belongs to the region corresponding to the index.

We find a solution to Equation (4) in region I with the boundary condition at the end of the string $R(0, \zeta) = 0$. But first, for computational convenience, we make the substitution on the right side of Equation (4) $\frac{\partial R}{\partial \zeta} = \frac{1}{s_0} \frac{\partial R}{\partial \xi}$, where

$s_0 = \frac{x_0}{t_0}$ —the disturbance velocity on the ED.

Such a substitution does not change the main form of the SG equation and follows from the identity obtained by dividing and multiplying the relative displacement of neighboring atoms at small time intervals and coordinates, for which we can take t_0 and x_0 . On the other hand, this substitution is equivalent to the string continuity condition.

To describe the ED motion at the FR source stage we consider the equation that follows from (4) after substitution $\frac{\partial R}{\partial \zeta}$ by $\frac{1}{s_0} \frac{\partial R}{\partial \xi}$ and rearrangement of terms:

$$\frac{\partial^2 R}{\partial \zeta^2} - \frac{\partial^2 R}{\partial \xi^2} = \Phi(\zeta) - \frac{\delta}{s_0} \frac{\partial R}{\partial \xi} - \sin(R). \tag{5}$$

To find a solution to (5) we perform substitution of variable ξ :

$$\xi = \frac{L}{2\pi} \vartheta, \tag{6}$$

where, $0 \leq \vartheta$ —the angle at the point of ED fixing counted counterclockwise from the axis ox .

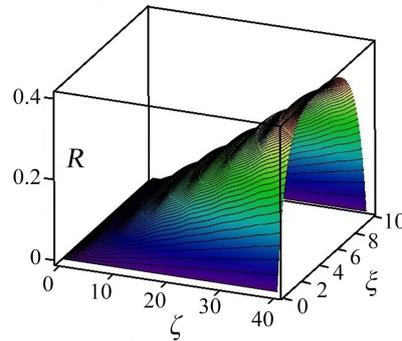


Figure 2. Formation of a semicircle from ED at the initial stage of the external stress. Units of the numbers on axis defines from (4).

It is easy to see that the solution of Equation (5) is the function:

$$R = A(\zeta + \zeta_0)\vartheta + B\zeta, \quad (7)$$

where, A, B, ζ_0 — constants defined by the condition of the problem.

The solution (7) describes the Archimedes spiral [27] and is valid under the condition $|A\zeta_0| \gg 1$ that corresponds to sufficiently high amplitudes of ED deviation from the initial position. This solution trivially satisfies the left side of Equation (5), and the right side determines the dependence of the external stress on the time:

$$\Phi(\zeta) = A \frac{2\pi\delta}{Ls_0} (\zeta + \zeta_0) - \sin(A(\zeta + \zeta_0)\vartheta + B\zeta). \quad (8)$$

where, A, B — constants.

Under the condition $|A| \frac{2\pi\delta}{Ls_0} \zeta_0 \gg 1$ the Peierls barrier is not a deterrent and the last term in the expression (8) can be omitted.

Thus, from the form of the solution (7) we can conclude that at $A > 0$ the external force $\Phi(\zeta)$ is an increasing with time magnitude. So, we assume further that the constant A is positive: $A > 0$.

Let us describe the temporal dynamics of a spiral in the Cartesian coordinate system, assuming $B < 0$. To do this, we normalize (7) so, that the radius of the Archimedes spiral is equal to unity.

$$r = \frac{R}{A(\zeta + \zeta_0)} = \vartheta - \frac{|B|}{|A|} \frac{\zeta}{\zeta + \zeta_0}. \quad (9)$$

At a zero time ($\zeta = 0$) the curve $r = \vartheta$ should be set in the form of a left spiral, since in this case the spiral shape within the interval $0 \leq \xi \leq 2\xi_{FR}$ is close to the shape of a semicircle (see **Figure 3**).

In parametric variables:

$$X = r \cos\left(\vartheta - \frac{\pi}{2}\right), \quad Y = -r \sin\left(\vartheta - \frac{\pi}{2}\right), \quad (10)$$

The segment of the Archimedes spiral described the position of the ED at $\zeta = 0$ is presented in **Figure 3**. Here, the ED initial position is marked by the

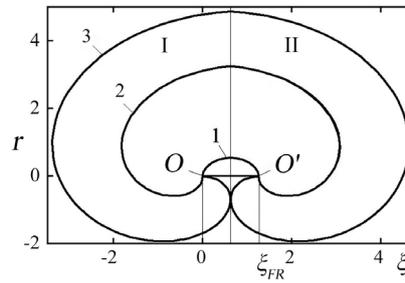


Figure 3. ED operation in FR source mode. Units of the numbers on axis defines from (4) and (10). Curve 1—ED at time $\zeta^* = 0$, angle of spiral rotation $\mathcal{G}^* = 0$; curve 2— $\zeta^* = 0.667$, angle of spiral rotation $\mathcal{G}^* = \pi$; curve 3— $\zeta^* = 1.5$, angle of spiral rotation $\mathcal{G}^* = 1.5\pi$.

digit 1 and described by the left Archimedes spiral displaced counterclockwise relative to $\mathcal{G} = 0$ at an angle $\pi/2$.

Over time the angle of spiral counterclockwise displacement increases and by the time $\zeta^*/\zeta_0 = \chi/(1-\chi)$ where, $\chi = \mathcal{G}^*/\alpha\pi < 1$ takes the value \mathcal{G}^* where, $0 < \mathcal{G}^* < 2\pi$.

Figure 3 shows ED successive positions at different points of time ζ^*/ζ_0 calculated for the values of constants: $\zeta_0 = 1$, $\alpha = 2.5$.

The transition to actual dimensions of the Archimedes spiral is carried out by multiplying the spiral (9) by a large factor $A(\zeta^* + \zeta_0)$.

Thus, in this section for the first time a particular solution of the SG equation is proposed, which describes the temporal dynamics of half the ED segment, counting from the stopper at the origin, in the FR source operating mode. Due to the symmetry of the problem a particular solution for the first half of the ED segment, which is mirrored relative to the axis of symmetry passed through the middle of the ED segment, describes also the behavior of the second half of the ED segment. For a horizontally located ED the proposed particular solution has the form of the left Archimedes spiral displaced counterclockwise by $\pi/2$ relative to the azimuth angle equal to zero. A graphic representation of the temporal dynamics of the found particular solution was plotted in the Cartesian coordinate system. It is shown that the proposed particular solution of SG equation for ED at FR source stage involves two Archimedes spirals symmetrical relative to the ED symmetry axis with radii increasing linearly with time and rotating towards each other relative to stoppers.

5. Conclusions

For the first time a particular analytical solution of the inhomogeneous dissipative sine-Gordon (SG) equation describing the ED temporal dynamics in the mode of FR source operation was obtained in this paper.

To do this, it was proposed to divide the process of the external force action on ED into two stages, where in the first stage the level of force action was less than critical, in the second—more.

At the first stage it is shown by numerical calculations of the SG equation that

the ED takes a shape close to semicircle for the external force value below the critical.

At the second stage of the force action the obtained calculation result of the first stage was used qualitatively as the initial condition of the SG equation to describe the ED temporal dynamics in the FR source operation mode. At a specified choice of the initial condition a particular solution of the SG equation is proposed to describe the ED temporal dynamics in the FR source operation mode. This particular solution describes the temporal dynamics of half of the ED, which rests on a stopper at the origin. The proposed particular solution for the initially horizontally located ED corresponds to the left Archimedes spiral displaced counterclockwise at $\pi/2$ relative to the azimuth angle equal to zero.

The temporal dynamics of the half of the ED segment rested on the second stopper is described by the proposed particular solution, when it is mirrored relative to the problem symmetry axis and the center of the spiral is displaced to a point with zero azimuthal angle and radius equal to the distance between the stoppers. The symmetry axis is a straight line that is perpendicular and divides in half the distance between the stoppers.

A graphic description of the ED temporal dynamics based on the proposed particular solution and its mirror and displaced image was plotted in the Cartesian coordinate system. It is shown that the particular solution of the SG equation in the RF source operation mode involves two Archimedes spirals symmetrical relative to the problem symmetry axis with equal radii increasing linearly with time, which rotate: one (the center of the spiral coincides with the stopper at the origin)—counterclockwise, the second (the center of the spiral coincides with the second stopper)—clockwise.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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