Spatial localization of nonlinear waves spreading in materials in the presence of dislocations and point defects

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Abstract. Within the framework of self consistent dynamic problems, the impact of dislocations and point defects on the spatial localization of nonlinear acoustic waves propagating in materials has been studied.

1. Introduction
The experimental data accumulated to this date allows us to state that dislocations and point defects have a significant influence on the propagation of acoustic waves in a solid. The role of dislocations is particularly important in the propagation of waves in a deformed or cyclically loaded body [1 - 3]. Theoretical description of the propagation of an acoustic wave in a solid with a changing density of dislocations would allow us to approach the problem of estimating the real state of a material and predicting its residual resource.

When the laser radiation or particle flux (e.g. in ion implantation) are exposed to the material it leads to creation of point defects (vacancies, interstices) [4]. The transmitting of an intense longitudinal acoustic waves facilitates the change in areas of tension and compression, the activation energy of formation of point defects, leading to their spatial redistribution. Defects migrating in material, recombine at various centers. The role of such centers can play a dislocation, impurity introduction, etc.

The aim of the paper is to study nonlinear self-consistent problems about the propagation of acoustic waves, taking into account their interaction with dislocations and point defects which are existed in the material.

2. Dislocation displacement solitons.
To take into account the interaction of dislocations with the lattice of the crystal, as well as the interaction of dislocations with one another, a mathematical model was proposed in [5, 6]:

\[ \frac{\partial^2 U}{\partial t^2} - c^2 \frac{\partial^2 U}{\partial x^2} = \frac{\beta \partial^2 \xi}{\rho \partial x}, \]  \hspace{1cm} (1)

\[ A \frac{\partial^2 \xi}{\partial t^2} + B \frac{\partial \xi}{\partial x} = -\beta \frac{\partial U}{\partial x}. \]  \hspace{1cm} (2)

Here \( U \) – acoustic displacement, \( \xi \) – dislocation displacement, \( A \) – mass of dislocations, \( B \) – frictional force per unit length of dislocation, \( \rho \) – density of a material, \( \beta = \beta_{ji} \cdot b_j \) – coefficient of
acoustic dislocation interaction (where \( \beta_{ijkl} \) – tensor of acoustic dislocation interaction, \( b_j \) – Burgers’ vector). In this case, the pulsation component will be assumed to be proportional to the square of the dislocation displacement \( \xi \) [5]: \( A = A_0 \left( 1 + A_1 \xi^2 \right) \), \( B = B_0 \left( 1 + B_1 \xi^2 \right) \), then the equation (2) will take the following form:

\[
\frac{\partial^2}{\partial t^2} U - c^2 \frac{\partial^2}{\partial x^2} U = \beta \frac{\partial}{\partial x} \xi ,
\]

\[
A_0 \left( 1 + A_1 \xi^2 \right) \frac{\partial^2}{\partial t^2} \xi + B_0 \left( 1 + B_1 \xi^2 \right) \frac{\partial}{\partial t} \xi = -\beta \frac{\partial}{\partial x} U
\]  \( \text{(3)} \)

Assuming, at the first stage of the investigation, the dislocation subsystem to be conservative \((B_0 = 0)\), let us rewrite (3) in the form of the one equation:

\[
\frac{A_0}{\beta} \frac{\partial^4}{\partial t^4} \xi - \frac{c^2 A_0}{\beta} \frac{\partial^4}{\partial x^2 \partial t^2} \xi - \frac{\beta}{\rho} \frac{\partial^2}{\partial x^2} \xi + \frac{A_0 A_1}{\beta} \left( \frac{\partial^2}{\partial t^2} - \frac{c^2 \partial^2}{\partial x^2} \right) \left( \xi^2 \frac{\partial^2}{\partial t^2} \xi \right) = 0
\]  \( \text{(4)} \)

which describes the propagation of the dislocation displacement wave.

Equation (4) has solutions in the form of traveling nonlinear stationary waves propagating with a constant velocity \((V = \text{const})\).

If the material possesses positive nonlinearity \((A_1 > 0)\), then dislocation displacements solitons might form in it.

In the subsonic range of the velocity \((V < c)\) the form of the soliton is described with hyperbolic secant:

\[
\xi = A_c \sec h \left( \frac{x - Vt}{\Delta} \right)
\]  \( \text{(5)} \)

and represents localized bell-shaped perturbation having a positive polarity. The width of the soliton is determined by the effective mass per unit dislocation length \((A_0)\) and by the coefficient of acoustic dislocation interaction \((\beta)\), i.e.

\[
\Delta \sim \sqrt{A_0}, \Delta \sim 1/\beta ,
\]  \( \text{(6)} \)

while the amplitude is defined by the nonlinearity parameter \( A_c = \sqrt{2/A_1} \).

In the supersonic range of velocity \((V < c)\) the form of the soliton is described with hyperbolic tangent:

\[
\xi = A_c \tanh \left( \frac{x - Vt}{\Delta} \right)
\]  \( \text{(7)} \)
and represents the step between two constant values \( \xi_+ \) and \( \xi_- \). Such a soliton is called “kink”, it is analogous to a shock wave whose front width is determined by the relations (5), and the amplitude (the magnitude of the drop) is equal to \( A_c = \sqrt{1/A_i} \).

In materials which possess a negative dislocation nonlinearity \( (A_i < 0) \) solitons cannot be formed, only periodic nonlinear stationary waves can propagate in such materials.

Let us estimate the influence of the nonconservativity of the dislocation subsystem on the wave processes.

If the dislocations are assumed to be free-inertial \( (A_0 = 0) \), then the system (3) can be reduced to the equation:

\[
\frac{d^2 \xi}{d\eta^2} = \frac{\beta^2 \xi}{\rho^2 V(V^2 - c^2)B_i(1 + B_i \xi^2)}
\]  

(8)

where \( \eta = x - Vt \), which take the following form when \( (B_i \xi^2 << 1) \):

\[
\frac{d\xi}{d\eta} + \alpha \xi - \alpha B_i \xi^3 = 0,
\]  

(9)

where \( \alpha = \frac{\beta^2}{\rho^2 B_i V(c^2 - V^2)} \).

The solution to the equation (9) we will look in the form \( \xi = \xi_0 e^{ik\eta} + \xi_0^* e^{-ik\eta} \), where \( k = k' + ik'' \) – complex wavenumber, \( \xi_0 \) – complex amplitude, \( \xi_0^* \) – complex conjugate amplitude.

Neglecting the higher harmonics and taking into account the contribution of the nonlinearity only to the fundamental harmonic, we obtain:

\[
k' = 0, \\
k'' = \alpha (1 - 3B_i|\xi_0|^2).
\]  

(10)

During the propagation of a supersonic wave \( (c < V) \) exponential damping occurs, besides a "soft" nonlinearity, i.e. when \( (B_i < 0) \) the nonlinear wave decays faster than the linear wave. With a "hard" nonlinearity, i.e. when \( (B_i > 0) \) the linear wave decays faster than the nonlinear one.

During the propagation of a subsonic wave \( (c > V) \) the dislocation viscosity leads to an increase in the amplitude of the wave, i.e. the system behaves as an active one. For a "soft" nonlinearity, a nonlinear wave grows faster than a linear wave, for a "hard" nonlinearity, a linear wave grows faster than a linear wave.

3. Point defects

In [7, 8] it is shown that the problem of propagation of acoustic wave in the material with defects, should be considered as self-consistent, comprising along with a dynamic equation of elasticity theory, the kinetic equation for the density of defects:

\[
\frac{\partial^2 u}{\partial t^2} - c_i^2 \frac{\partial^2 u}{\partial x^2} - \frac{\beta_N}{\rho} \frac{\partial u}{\partial x} \frac{\partial^2 u}{\partial x^2} = -\left(\frac{\lambda + \frac{2}{3}\mu}{\rho}\right) \frac{\partial n_j}{\partial x}
\]  

(11)
\[ \frac{\partial n_j}{\partial t} = q_0 + q_x \frac{\partial u}{\partial x} + D_j \frac{\partial^2 n}{\partial x^2} - \beta_j n_j \]  \hspace{1cm} (12)

Here \( u(x,t) \) – longitudinal dislocation material particles (the wave is considered flat); \( n_j(x,t) \) – volume concentration of point defects; \( j = v \) – for vacancies, \( j = i \) – for interstices; \( c_i = \sqrt{\lambda + 2\mu}/\rho \) – the velocity of the longitudinal wave propagation in the material, in the case of absence of defects; \( \lambda, \mu \) – Lame modulus; \( \rho \) – density of the material; \( \beta_N \) – nonlinearity coefficient: \( \beta_N = 3\lambda + 6\mu + 2A + 6B + 2C; \) \( A, B, C \) – Landau modulus of the third order; \( \Omega_j \) – dilatational parameter which characterizes the volume change when a single point defect appears (for vacancies \( \Omega_j < 0 \), for interstices \( \Omega_j > 0 \)).

Equation (12) is written under the assumption that the main processes determining the behavior of the defects are the processes of generation, recombination and diffusion. Through \( q_0 \) it is denoted the rate of generation of point defects in the absence of deformation; the second term in the right part of (12) is a deformation correction to the generation of defects; \( D_j \) – diffusion coefficient of defect of type \( j \); \( \beta_j \) – recombination velocity on the effluent. Volume of mutual recombination of unlike defects is not taken into account.

The system (11), (12) can be reduced to a single nonlinear equation with respect to displacement:

\[
\frac{\partial^2 u}{\partial t^2} - \left( \frac{c_i^2}{\rho \cdot \beta_j} \right) \frac{\partial^2 u}{\partial x^2} \left( \frac{\partial^2 u}{\partial x^2} + D_j \frac{\partial^4 u}{\partial x^4} \right) - \frac{1}{\beta_j} \left( \frac{\partial^3 u}{\partial x^3} - c_i^2 \frac{\partial^3 u}{\partial x^3} \right) = \frac{\beta_N}{2\rho} \left[ \frac{\delta (\frac{\partial u}{\partial x})^2}{\beta_j \frac{\partial^3 x}{\partial x}} - D_j \frac{\partial^5 x}{\partial x^5} \left( \frac{\partial u}{\partial x} \right)^2 + 1 \frac{\partial^2 x}{\partial x^2} \left( \frac{\delta u}{\delta x} \right)^2 \right]
\]  \hspace{1cm} (13)

Let us introduce dimensionless displacement, coordinate and time:

\[
\tilde{U} = \frac{U}{U_0}, \tilde{x} = x \sqrt{\frac{\beta_j}{D_j}}, \tilde{t} = t \left( \frac{\beta_j}{D_j} \right)^{\frac{1}{2}} \left( \frac{\rho \cdot c_i^2}{\rho \cdot \beta_j} \right)^{\frac{1}{2}} - q_x \left( \lambda + \frac{2}{3} \mu \right) \Omega_j
\]  \hspace{1cm} (14)

Then equation (13) can be transformed to the following form:

\[
\frac{\delta^2 \tilde{U}}{\delta \tilde{t}^2} - \frac{\delta^2 \tilde{U}}{\delta \tilde{x}^2} - \frac{\delta^4 \tilde{U}}{\delta \tilde{x}^4} + 1 \frac{\delta^4 \tilde{U}}{\delta \tilde{x}^4} + b \sqrt{a} \left( \frac{\delta^3 \tilde{U}}{\delta \tilde{t}^3} - 1 \frac{\delta^3 \tilde{U}}{\delta \tilde{x}^3} \right) = \frac{\beta_N}{2\rho} \left[ \sqrt{\frac{\beta_j}{D_j}} U_0 \left( \frac{\delta \tilde{U}}{\delta \tilde{x}} \right)^2 - \frac{\delta^3 \tilde{U}}{\delta \tilde{x}^3} \left( \frac{\delta \tilde{U}}{\delta \tilde{x}} \right)^3 \right] + \frac{U_0}{D_j c_i^2 a} \frac{\delta^2 \tilde{U}}{\partial \tilde{x} \partial \tilde{t}} \left( \frac{\delta \tilde{U}}{\delta \tilde{x}} \right)^2
\]  \hspace{1cm} (15)
Here we introduced the following designations

\[ a = 1 - \frac{2}{3} \frac{\mu}{\beta_j \rho^2_i}, \quad b = \frac{c_i}{\sqrt{\beta_j^* D_j}}. \]

In the linear approximation, \( \beta_N = 0 \) the equation (15) has the following form:

\[
\frac{\partial^2 \tilde{U}}{\partial t^2} - \frac{\partial^2 \tilde{U}}{\partial x^2} = \frac{\partial^4 \tilde{U}}{\partial x^2 \partial t^2} + \frac{1}{a} \frac{\partial^4 \tilde{U}}{\partial x^4} + b \sqrt{a} \left( \frac{\partial^3 \tilde{U}}{\partial x \partial t^3} - \frac{1}{a} \frac{\partial^3 \tilde{U}}{\partial x^3 \partial t} \right) = 0 \tag{16}
\]

Looking for the solution of equation (16) in the form of traveling harmonic wave:

\[ U = A_0 e^{i(\omega t - kx)} + A_0^* e^{-i(\omega t - kx)}, \tag{17} \]

where \( \omega \) - the frequency; \( k = \frac{2\pi}{\Lambda} \) - the wave number (\( \Lambda \) - the wavelength); \( A_0^* \) - complex amplitude (\( A_0 \) - its complex-conjugate value), we get the following dispersion equation:

\[ k^4 - k^2(a - a \omega^2 + i b \sqrt{a} \omega) + a(\omega^2 + i b \sqrt{a} \omega^3) = 0. \tag{18} \]

Note that in equation (18), spatial and time scales of the longitudinal wave, contains complex coefficients, which implies that the wave will not only spread in the medium, but also to fade along with propagation.

Firstly, consider the special case, when \( b = 0 \), this is possible if the diffusion coefficient to tend to infinity \( (D_j \to \infty) \). Then the coefficients of the dispersion equation (18) will be real and it will look like:

\[ k^4 - k^2(a - a \omega^2) + a \omega^2 = 0. \tag{19} \]

The frequency and wave number are related by:

\[ \omega = \pm k \sqrt{\frac{1 - \frac{1}{a} k^2}{1 + k^2}}, \tag{20} \]

i.e., the presence of point defects leads to the dispersion of longitudinal elastic waves. The graph of (20) determines the dispersion curve in the plane \((\omega, k)\). The curve at small wave numbers has the asymptote \( \omega = k \), and for large – asymptotically approaches a straight line \( \omega = \sqrt[3]{a}. \)

Phase velocity of the wave is determined by the formula:

\[ V_{ph} = \frac{\omega}{k} = \pm \sqrt{\frac{1 - \frac{1}{a} k^2}{1 + k^2}}. \tag{21} \]
and the group velocity is associated with it by the ratio (Rayleigh):

$$V_{gr} = V_{ph} + k \frac{dV_{ph}}{dk}.$$  \hspace{1cm} (22)

When \( k \to 0 \) phase velocity \( V_{ph} \to 1 \), when \( k \to \infty \) \( V_{ph} \to \frac{1}{\sqrt{a}} \). If point defects are vacancies \((j = v)\), then \( \Omega_j < 0 \), consequently \( \frac{1}{\sqrt{a}} < 1 \) and dispersion in this case is normal \( (V_{ph} > V_{gr}) \). If point defects are interstices \((j = i)\), then \( \Omega_j > 0 \), consequently \( \frac{1}{\sqrt{a}} > 1 \) and dispersion is abnormal \( (V_{ph} < V_{gr}) \).

When \( b \neq 0 \), i.e. when the values of the diffusion coefficients \( (D_j) \) are finite, the wave number in the study of the dispersion equation \( (18) \) can be written in the form \( k = k' + ik'' \), where \( k' \) characterizes the propagation constant \( \left( V_{ph} = \frac{\omega}{k'} \right) \) - phase velocity of the wave, but \( k'' = \alpha(\omega) \) characterizes the wave attenuation.

Longitudinal wave in a medium with point defects is dispersive and damped along its propagation. Attenuation has an extreme character.

Returning to the study of nonlinear equation \( (15) \), let us assume that the dispersion and attenuation of waves due to the presence of point defects, and the nonlinearity of the material is the value of the same order of smallness. The solution of equation \( (15) \) is looking in the form of the asymptotic expansion of displacement in the small parameter:

$$\tilde{U} = U_0 + \varepsilon U_1 + ...$$ \hspace{1cm} (23)

And introduce new variables:

$$\tilde{\xi} = \tilde{x} - c \tilde{t}; \eta = \varepsilon \tilde{\xi}$$ \hspace{1cm} (24)

This choice of variables is explained by the fact that the perturbation propagating with the velocity along the axis \( \tilde{x} \), slowly evaluates in space due to the nonlinearity, dispersion and dissipation. After substituting \( (23) \) and \( (24) \) in \( (15) \) in the zero approximation of \( \varepsilon \) it is obtained the expression for the velocity \( c = 1 \) that matches the velocity \( c_i \) in dimensional variables.

The first approximation on \( \varepsilon \) gives the evolutionary equation with respect to axial deformation

$$W = \frac{\partial U_0}{\partial \xi}; \hspace{1cm} \frac{\partial W}{\partial \eta} + \left( a - 1 \right) \frac{\partial^3 W}{\partial \xi^3} + \frac{b(a - 1)}{2a} \frac{\partial^2 W}{\partial \xi^2} + q W \frac{\partial W}{\partial \xi} = 0,$$ \hspace{1cm} (25)

where \( q = \beta_N \sqrt{\beta_j U_0} / \sqrt{2 \rho \sqrt{D_j c_i^2 a}} \). Equation \( (25) \) is called the Korteweg-de Vries-burgers. It has a solution in the form of a localized wave (a kink):
\[ W = A_0 \exp \left( \frac{-\xi}{2} \right) \sec \left( \frac{\xi}{2} \right), \xi = \frac{2}{\Delta} (\xi - V \eta) \] (26)

Here \( A_0 \) - the amplitude of the wave, \( V \) - its velocity, \( \Delta \) - the characteristic width. Their values are determined by the expressions:

\[ A_0 = \frac{3c_i^j \left[ -q_e \left( \lambda + \frac{2}{3} \mu \right) \Omega_j \right]}{25 \beta_j^2 \sqrt{\beta} \left[ \left(-\beta \right) \frac{\sqrt{D_j}}{U_0} \right]}, \] (27)

\[ V = \frac{3q_e \left( \lambda + \frac{2}{3} \mu \right) \Omega_j}{25 \beta_j^2 D_j \rho} \times \Delta = \frac{10 \sqrt{\beta_j D_j}}{c_i \left[ 1 \frac{q_e \left( \lambda + \frac{2}{3} \mu \right) \Omega_j}{\beta_j \rho c_i^j} \right]}. \] (28)

In the relations (27) – (28) \( \frac{q_e \left( \lambda + \frac{2}{3} \mu \right) \Omega_j}{\beta_j \rho c_i^j} < 1 \), consequently for estimations the following formulas are valid:

\[ A_0 \approx \frac{-3c_i^j q_e \left( \lambda + \frac{2}{3} \mu \right) \Omega_j}{25 \beta_j^2 \sqrt{\beta} \left[ \left(-\beta \right) \frac{\sqrt{D_j}}{U_0} \right]}, \Delta \approx \frac{10 \sqrt{\beta_j D_j}}{c_i}. \] (29)

Equation (26) describes the stationary wave profile. Such waves are formed by a joint of a balance between nonlinearity, dispersion and dissipation. Consequently, the presence of point defects in the material affects the process of localizing the propagation of strain waves. If point defects are vacancies \((j = v)\), then the wave profile represents the difference (“step”) from highest to lowest. If point defects are the interstices \((j = i)\), then the wave profile is the difference from lowest to highest. For both types of defects the amplitude of the wave decreases with increasing recombination rate at drains as \( A_0 \sim 1/\beta_j^2 \), its velocity decreases as \( V \sim 1/\beta_j^2 \), but width increases as \( \Delta \sim \sqrt{\beta_j} \). This behavior is the same wave parameters and with the growth of the diffusion coefficient: the amplitude and speed decrease \( A \sim 1/\sqrt{D_j}, V \sim 1/D_j \), but width increases \( \Delta \sim \sqrt{D_j} \).

4. Conclusions

Expressions are obtained that describe the dependence of the dislocation displacement soliton width on the effective mass per unit length of the dislocation, and the coefficient of acoustic dislocation interaction.

It is shown that the interaction of a nonlinear deformation wave with the field of concentration of point defects (vacancies, interstices) leads both to wave scattering and to a change in the activation energy of defect formation and their spatial redistribution.
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