Generalized susceptibility of a screw dislocation in ferroelastics near structural phase transition

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Abstract. Small amplitude bending vibrations of a screw dislocation near structural phase transition is considered. Based on the full set of equations describing the vibrations of a crystal with a dislocation near the structural phase transition, written equations for the dynamics of screw dislocations in the linear approximation of the dislocation displacement. Fourier transform of the Peach-Koehler forces projection on the dislocation slip plane is obtained and a linear response function of a screw dislocation in ferroelastic crystal to an external force is found.

1. Introduction
It is known that in the vicinity of the structural phase transition almost all physical properties behave abnormally [1-3]. The interest in studying the vicinity of the structural phase transition point is also due to the fact that the system in this region is very compliant to external perturbations affecting the order parameter \( \eta \) [4]. The presence of defects affects the anomalous behavior of the physical properties in the vicinity of the structural phase transition [5]. Previously, a dislocation that was stationary and moving at a constant speed in the vicinity of the structural phase transition was considered [6-18]. Bending vibrations of dislocations were not discussed in these papers. Dislocation bending vibrations in non-ferroelastic crystals using the self-consistent dynamic theory of dislocations in [19, 20] were considered. In [21, 22], the exact solution of the problem of finding edge dislocation generalized susceptibility in a crystal with a soft mode is given in the framework of the linear theory of elasticity and Landau's phenomenological theory of phase transitions [4]. In [23–26], the generalized susceptibility of edge and screw dislocations in ferroelectric was found. In the present work we study the screw dislocation bending vibrations and find the screw dislocation generalized susceptibility in the vicinity of structural phase transition.

2. Set of equations, describing screw dislocation vibrations in ferroelastic crystal
We believe that the presence of a dislocation leads to the appearance of an addition \( \eta_1(r,t) \) to the thermodynamically equilibrium value of the order parameter \( \eta_e \). Addition \( \eta_1(r,t) \) in the general case depends on both coordinates \( r \) and time \( t \). We write the complete system of equations (1)-(4) describing the vibrations of a ferroelastic crystal with a dislocation [21, 22]:

\[
f_k = e_{ikl} \tau_l \sigma_{lm} b_m = 0,
\]

where \( f \) is Peach-Koehler force, \( e_{ikl} \) is Levi-Civita symbol, \( \tau \) is vector of the tangent to the dislocation line, \( \sigma_{lm} \) is stress tensor, and \( b \) is Burgers vector. It is more convenient to use
projection of this force onto the slip plane \( f_\perp = n_\sigma l m b_m \), where \( n \) is normal vector to the slip plane of the dislocation.

\[
\frac{1}{c_i^2} \frac{\partial^2 f_\perp}{\partial t^2} - \nabla^2 f_\perp + \frac{3n_\beta_j}{1 + \nu} \frac{\partial^2 p}{\partial x_j \partial x_j} - 2\mu g (n \cdot \nabla) (b \cdot \nabla) (\eta_s \eta_1) = - \rho b^2 \frac{\partial V}{\partial t} \delta(\xi) - 2\mu n_\beta b_k \eta_{ik}. \tag{2}
\]

Here \( c_i \) is velocity of transverse sound waves, \( \nu \) is Poisson's ratio, \( \mu \) is shear modulus, \( g \) is constant striction coefficient, \( \rho \) is density of the crystal substance, \( V \) is velocity of the dislocation line at this point, \( \delta(\xi) \) is two-dimensional \( \delta \)-function, \( \xi \) is two-dimensional radius vector, counted from the axis of dislocation in a plane perpendicular to the vector \( \tau \),

\[
\eta_{ik} = e_{jke} \frac{\partial}{\partial x_j} \left[ (\tau_i b_n - \frac{1}{2} \tau b_\delta_{ik}) \delta(\xi) \right]
\]
is deformation incompatibility tensor [27].

\[
\frac{1}{c_i^2} \frac{\partial^2 p}{\partial t^2} - \nabla^2 p + \frac{4}{3} \frac{\mu}{1 - \nu} \left[ \frac{1}{c_i^2} \frac{\partial^2 (\eta_s \eta_1)}{\partial t^2} - \nabla^2 (\eta_s \eta_1) \right] = - \frac{2}{3} \frac{\mu}{1 - \nu} \eta_{ii}, \tag{3}
\]
where \( c_i \) is velocity of longitudinal sound waves.

\[
\eta_1(r, t) = -3\eta_s g \int \chi(r - r', t - t') p(r', t') \, dr' \, dt'. \tag{4}
\]

Here \( \chi = \chi(r,t) \) is function of the order parameter response to the hydrostatic pressure \( p \).

We choose a coordinate system so that the dislocation line is located along the axis \( Oz \), \( \tau = (0, 0, -1) \), \( b = (0, 0, b) \), \( n = (0, 1, 0) \). Considering the small amplitudes of dislocation vibrations near the equilibrium position and limited to a linear approximation with respect to the dislocation displacement \( u = u(z, t) \), we obtain

\[
\tau = \left( -\frac{\partial u}{\partial z}, 0, -1 \right), \quad \delta(\xi) = \delta(x) \delta(y) - \delta'(x) \delta(y) u,
\]

\[
\frac{\partial V}{\partial t} \delta(\xi) = \frac{\partial^2 u}{\partial t^2} \left( \delta(x) \delta(y) - \delta'(x) \delta(y) u \right) \approx \frac{\partial^2 u}{\partial t^2} \delta(x) \delta(y),
\]

\[
f_\perp = n_\sigma l m b_m = \sigma_{yz} b, \quad (n \cdot \nabla)(b \cdot \nabla)(\eta_s \eta_1) = b \eta_s \frac{\partial^2 \eta_1}{\partial y \partial z},
\]

\[
n_1 \eta_{ik} b_k = b \eta_{yz} = \frac{1}{2} b^2 \left( \delta'(x) \delta(y) - \delta''(x) \delta(y) u \right), \quad \eta_{ii} = - b \frac{\partial u}{\partial z} \delta(x) \delta'(y).
\]

Thus, equations (2) and (3) take the form

\[
\frac{1}{c_i^2} \frac{\partial^2 f_\perp}{\partial t^2} - \nabla^2 f_\perp + \frac{3b}{1 + \nu} \frac{\partial^2 p}{\partial y \partial z} - 2\mu g b \eta_s \frac{\partial^2 \eta_1}{\partial y \partial z}
\]

\[
= -\rho b^2 \frac{\partial^2 u}{\partial t^2} \delta(x) \delta(y) - \mu b^2 \left[ \delta'(x) \delta(y) - u \delta''(x) \delta(y) \right], \tag{5}
\]
\[
\frac{1}{c_i^2} \frac{\partial^2 \rho}{\partial t^2} - \nabla^2 \rho + \frac{4+1+v}{3(1-v)} \mu g \eta_i \left( \frac{1}{c_i^2} \frac{\partial^2 \eta_1}{\partial t^2} - \nabla^2 \eta_1 \right) = \frac{2(1+v)}{3(1-v)} \mu b \frac{\partial u}{\partial z} \delta(x) \delta'(y) .
\]

Equations (4)-(6) with the boundary condition (1) represent the complete system of equations describing the vibrations of a crystal with a screw dislocation near the structural phase transition.

3. Generalized susceptibility of screw dislocation

We perform the Fourier transform for the system of equations (4)-(6) with respect to the variables \( r \) and \( t \):

\[
\tilde{\eta}_1 = -3g \eta_j \tilde{\chi},
\]

\[
(q^2 - \omega^2/\epsilon_i^2) \tilde{f}_{\perp} - \frac{3b}{1+v} q_x q_z \tilde{p} + 2 \mu b g \eta_j q_x q_z \tilde{\eta}_1 = -\mu b^2 (q_x^2 - \omega^2/\epsilon_i^2) \tilde{u} - i(2\pi)^2 \mu b^2 q_x \delta(q_z) \delta(\omega),
\]

\[
(q^2 - \omega^2/\epsilon_i^2) \tilde{p} + \frac{4+1+v}{3(1-v)} \mu g \eta_j (q^2 - \omega^2/\epsilon_i^2) \tilde{\eta}_1 = \frac{2(1+v)}{3(1-v)} \mu b q_z \tilde{u}.
\]

Here \( \tilde{\eta}_1(q,\omega), \tilde{\chi}(q,\omega) = \tilde{\chi}_0 \omega_0^2 (\omega_0^2 + \kappa q^2 - \omega^2) \) [1], \( \tilde{p}(q,\omega), \tilde{f}_{\perp}(q,\omega), \tilde{u}(q,\omega) \) are the Fourier transforms, \( q \) is wave vector, \( \omega \) is frequency, \( \omega_0^2 = a |T - T_c| \) is square of soft mode characteristic frequency, \( T_c \) is temperature of the structural phase transition, \( \kappa \sim \epsilon_i^2 \). We find the projection of the Peach-Koehler force by solving the system of equations (7)-(9).

\[
\tilde{f}_{\perp}(q,\omega) = -\mu b^2 \frac{2q_x^2 q_y^2 \left( 1 + (1+v) \mu g^2 \eta_j \tilde{\chi} \right)}{(1-v) (q^2 - \omega^2/\epsilon_i^2) (q^2 - \omega^2/\epsilon_i^2) - 4(1+v) \mu g^2 \eta_j \tilde{\chi} (q^2 - \omega^2/\epsilon_i^2)^2} \tilde{u} - \mu b^2 \frac{q_x^2 - \omega^2/\epsilon_i^2}{q^2 - \omega^2/\epsilon_i^2} \tilde{u} - i(2\pi)^2 q_x \delta(q_z) \delta(\omega) \frac{q^2 - \omega^2/\epsilon_i^2}{q^2 - \omega^2/\epsilon_i^2} .
\]

Using expression (10), we find the projection of the Peach-Koehler force onto the dislocation line \((x = 0, y = 0)\). For this, we perform the inverse Fourier transform of the expression (10) with respect to the variables \( q_x \) and \( q_y \), and then set \( x = y = 0 \):

\[
\tilde{f}_{\perp}(x,y,q_z,\omega) = \int_{-\infty}^{\infty} \tilde{f}_{\perp}(q,\omega) e^{i(q_x x + q_y y)} \frac{dq_x dq_y}{(2\pi)^2} ,
\]

\[
\tilde{f}_{\perp}(0,0,q_z,\omega) = \tilde{f}_{\perp}(q_z,\omega) = \int_{-\infty}^{\infty} \tilde{f}_{\perp}(q,\omega) \frac{dq_x dq_y}{(2\pi)^2} .
\]

Passing to the polar coordinates in (11) and performing integration over the polar angle, we obtain equation of screw dislocation bending vibrations \( \tilde{f}_{\perp}(q_z,\omega) = \alpha_D^{-1}(q_z,\omega) \tilde{u}(q_z,\omega) \), where \( \alpha_D(q_z,\omega) \) is the generalized susceptibility (linear response function) of the screw dislocation near the structural phase transition. For the inverse generalized susceptibility, the formula is obtained

\[
\alpha_D^{-1}(q_z,\omega) = -\frac{\mu b^2}{4\pi} \int q_z dq_z \frac{q_z^2 - 2\omega^2/\epsilon_i^2}{q_z^2 - \omega^2/\epsilon_i^2} .
\]
\[ + \frac{2q^2 q_z^2 \left( 1 + 2(1 + \nu) \mu \frac{\eta^2}{c_T^2} \right)}{(1 - \nu)(q^2 - \omega^2/c_T^2)(q^2 - \omega^2/c_T^2) - 4(1 + \nu) \mu \frac{\eta^2}{c_T^2} \omega^2} \] 

In the case of natural vibrations of dislocation \( \alpha^{-1}_D (q_z, \omega) = 0 \) should be assumed. From this equation, the eigenfrequencies of bending dislocation vibrations in the vicinity of the structural phase transition and their damping can be found. Using the expression for the generalized susceptibility, we can establish effect of an elastic field interaction with a soft mode on the effective mass and effective rigidity of a screw dislocation.

4. Conclusion
The obtained result can be used to study the attenuation and scattering of ultrasound and other external effects on a crystal with dislocations. It is known that ferroelastics are used in various optical, acoustoelectronic and electromechanical devices. We believe that the features of the characteristics of a screw dislocation in the vicinity of the structural phase transition, established in the work, are not only of scientific interest, but will also allow in some cases to optimize the parameters of devices based on ferroelastics.

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