Torsional Elastic Waves in Double Wall Tube

M. O. Katanaev *

Steklov Mathematical Institute,
ul. Gubkina, 8, Moscow, 119991, Russia

03 March 2015

Abstract

We describe the double wall tube with cylindrical dislocation in the framework of the geometric theory of defects. The induced metric is found. The dispersion relation is obtained for the propagation of torsional elastic waves in the double wall tube.

1 Introduction

Ideal crystals are absent in nature, and most of their physical properties, such as plasticity, melting, growth, etc., are defined by defects of the crystalline structure. Therefore, a study of defects is a topical scientific question of importance for applications in the first place. At present, a fundamental theory of defects is absent in spite of the existence of dozens of monographs and thousands of articles.

One of the most promising approaches to the theory of defects is based on Riemann–Cartan geometry, which involves nontrivial metric and torsion. In this approach, a crystal is considered as a continuous elastic medium with a spin structure. If the displacement vector field is a smooth function, then there are only elastic stresses corresponding to diffeomorphisms of the Euclidean space. If the displacement vector field has discontinuities, then we are saying that there are defects in the elastic structure. Defects in the elastic structure are called dislocations and lead to the appearance of nontrivial geometry. Precisely, they correspond to a nonzero torsion tensor, equal to the surface density of the Burgers vector. Defects in the spin structure are called disclinations. They correspond to nonzero curvature tensor, curvature tensor being the surface density of the Frank vector.

The idea to relate torsion to dislocations appeared in the 1950s [1–4]. This approach is still being successfully developed (note reviews [5–11]), and is often called the gauge theory of dislocations.

Some time ago we proposed the geometrical theory of defects [12–14]. Our approach is essentially different from others in two respects. Firstly, we do not have the displacement and rotational angle vector fields as independent variables because, in general, they are not continuous. Instead, the triad field and $\mathfrak{so}(3)$-connection are considered as independent variables. If defects are absent, then the triad and $\mathfrak{so}(3)$-connection reduce to partial

*E-mail: katanaev@mi.ras.ru
derivatives of the displacement and rotational angle vector fields. In this case the latter can be reconstructed. Secondly, the set of equilibrium equations is different. We proposed purely geometric set which coincides with that of Euclidean three dimensional gravity with torsion. The nonlinear elasticity equations and principal chiral $\mathbb{S}O(3)$ model for the spin structure enter the model through the elastic and Lorentz gauge conditions [14–16] which allow to reconstruct the displacement and rotational angle vector fields in the absence of dislocations in full agreement with classical models.

The advantage of the geometric theory of defects is that it allows one to describe single defects as well as their continuous distributions.

In the present paper, we consider propagation of torsional elastic waves in double wall tube with cylindrical dislocation. This defect was first described in [17]. The Schrödinger equation for the double wall tube was solved in [18] and applied to double wall nanotubes. A similar problem was also solved for the cylindrical waveguide with wedge dislocation [19].

1.1 Double wall tube

Let us describe double wall tube with cylindrical dislocation in the framework of the geometric theory of defects.

We consider cylindrical coordinates $\{x^\mu\} = \{r, \varphi, z\}$, $\mu = 1, 2, 3$ in tree dimensional Euclidean space $\mathbb{R}^3$. Let there be two thick tubes $r_0 \leq r \leq r_1$ and $r_2 \leq r \leq r_3$ of elastic media, each axis coinciding with the $z$ axis. We suppose that $r_0 < r_1 < r_2 < r_3$ (see Fig. 1a, where a section $z = \text{const}$ is shown). Now we make one tube with the inside cylindrical dislocation in the following manner. We stretch symmetrically the inner tube and compress the outer one. Then glue together the external surface of the inner tube with the internal surface of the outer tube. Afterwards the media comes to some equilibrium state. Due to rotational and translational symmetry we obtain one tube $r_\text{in} \leq r \leq r_\text{ex}$ with the axis which coincides with the $z$ axis (see Fig.1b). Radii of cylinders constituting tube surfaces are mapped as follows

$r_0 \mapsto r_\text{in}, \quad r_1, r_2 \mapsto r_*, \quad r_3 \mapsto r_\text{ex}.$

The gluing is performed along the cylinder $r_*$, and there is cylindrical defect (dislocation) because part of the media between tubes is removed.
The obtained double wall tube with cylindrical dislocation is rotationally and translationally symmetric.

The constructed model of the tube with cylindrical dislocation can be considered as continuous model of double wall nanotube (for a general review, see [20, 21, 22]). Consider double wall nanotube having two atomic layers. Suppose the inner layer has 18 and outer layer has 20 atoms which are shown in Fig. 1 by points. Natural length measure here is the interatomic distance. Then the length of a circle has a jump when one goes from inner to outer layer. In the geometric theory of defects, it means that the metric component $g_{\varphi\varphi}$ is not continuous in cylindrical coordinates. The corresponding model will be described below.

To find radii $r_{in}$, $r_*$, and $r_{ex}$ we have to solve the classical elasticity problem.

Let us define the displacement vector field by

$$y^i \mapsto x^i = y^i + u^i(x),$$  

where $y^i$ and $x^i$ are coordinates of a point before and after deformation respectively. We consider the displacement field as a vector function on points of media after deformation and gluing. This is more adequate because the resulting media after gluing is a connected manifold (before the gluing procedure, each tube represents a connected component). In equilibrium state, the vector displacement field satisfies equation

$$(1 - 2\sigma) \Delta u_i + \partial_i \partial_j u^j = 0,$$  

where $\sigma$ is the Poisson ratio and $\Delta$ is the Laplacian. For convenience, we consider components of the displacement vector field with respect to the orthonormal basis

$$u = u^r e_r + u^\varphi e_\varphi + u^z e_z,$$

where

$$e_r = \partial_r, \quad e_\varphi = \frac{1}{r} \partial_\varphi, \quad e_z = \partial_z.$$

We denote indices with respect to the orthonormal basis by hat:

$$\{i\} = \{\hat{r}, \hat{\varphi}, \hat{z}\}, \quad \{\mu\} = \{r, \varphi, z\}.$$  

The Latin indices referred to an orthonormal basis are rased and lowered by Kronecker symbol: $u_i := u^j \delta_{ji}$.

The divergence and Laplacian have the following form in cylindrical coordinates

$$\nabla_i u^i = \frac{1}{r} \partial_r (ru^r) + \frac{1}{r^2} \partial_\varphi u^\varphi + \partial_z u^z,$$

$$\Delta u_r = \frac{1}{r} \partial_r (ru_r) + \frac{1}{r^2} \partial_\varphi u_\varphi + \frac{1}{r^2} \partial_z u_z - \frac{1}{r^2} u_r - \frac{2}{r^2} \partial_\varphi u_\varphi,$$

$$\Delta u_\varphi = \frac{1}{r} \partial_r (ru_\varphi) + \frac{1}{r^2} \partial_\varphi u_\varphi + \frac{1}{r^2} \partial_z u_z - \frac{1}{r^2} u_\varphi + \frac{2}{r^2} \partial_\varphi u_\varphi,$$

$$\Delta u_z = \frac{1}{r} \partial_r (ru_z) + \frac{1}{r^2} \partial_\varphi u_\varphi + \frac{1}{r^2} \partial_z u_z.$$

From the symmetry of the problem, we deduce that only radial component of the displacement field differs from zero, and it does not depend on the angle $\varphi$ and $z$ coordinates:

$$\{u^i\} = \{u^r := u(r), u^\varphi = 0, u^z = 0\}.$$
Equation (2) for zero $u_\phi$ and $u_z$ components are automatically satisfied. It is easy to check that the radial derivative of the divergence,
\[
\partial_r \partial_j u^j = \partial_r \left( \frac{1}{r} \partial_r (ru) \right) = \partial_{rr}^2 u + \frac{1}{r} \partial_r u - \frac{1}{r^2} u,
\]
coincides with the Laplacian
\[
\triangle u_r = \frac{1}{r} \partial_r (r \partial_r u) - \frac{1}{r^2} u = \partial_{rr}^2 u + \frac{1}{r} \partial_r u - \frac{1}{r^2} u.
\]
Therefore the radial component of Eq.(2) takes the form
\[
\partial_r \left( \frac{1}{r} \partial_r (ru) \right) = 0. \tag{4}
\]
A general solution of this equation depends on two integration constants:
\[
u = c_1 r + \frac{c_2}{r}, \quad c_{1,2} = \text{const}.
\]
Note that the equilibrium equation (4) does not depend on the Poisson ratio $\sigma$. This means that the cylindrical dislocation is the geometrical defect.

Boundary conditions have to be imposed to fix the integration constants. Let us introduce notation for inner and outer tubes:
\[
u = \begin{cases} u_{\text{in}}, & r_{\text{in}} \leq r \leq r_*, \\ u_{\text{ex}}, & r_* \leq r \leq r_{\text{ex}}. \end{cases}
\]
Now boundary conditions are to be imposed. We assume that the surface of two wall nanotube is free, i.e. the deformation tensor is zero on the boundary:
\[
\left. \frac{du_{\text{in}}}{dr} \right|_{r=r_{\text{in}}} = 0, \quad \left. \frac{du_{\text{ex}}}{dr} \right|_{r=r_{\text{ex}}} = 0. \tag{5}
\]
We assume also that the media is in equilibrium. It means that elastic forces on the gluing surface must be equal to zero:
\[
\left. \frac{du_{\text{in}}}{dr} \right|_{r=r_*} = \left. \frac{du_{\text{ex}}}{dr} \right|_{r=r_*}. \tag{6}
\]
Each of boundary conditions (5) defines one integration constant for internal and external solutions:
\[
u_{\text{in}} = a \left( r + \frac{r_{\text{in}}^2}{r} \right) > 0, \quad a = \text{const} > 0,
\]
\[
u_{\text{ex}} = -b \left( \frac{1}{r} + \frac{r}{r_{\text{ex}}^2} \right) < 0, \quad b = \text{const} > 0. \tag{7}
\]
Signs of the integration constants $a$ and $b$ are chosen in such a way that displacement vector is positive and negative for inner and outer tubes respectively. This in agreement with the imposed problem.
Substitution of obtained solutions (7) into the gluing condition (6) defines the ratio of integration constants:

\[
r_*^2 = r_{ex}^2 \frac{ar_{in}^2 + b}{ar_{ex}^2 + b} \quad \Leftrightarrow \quad b = ar_{ex}^2 \frac{r_*^2 - r_{in}^2}{r_{ex}^2 - r_*^2}.
\] (8)

The entirety condition for the media is

\[
\begin{align*}
r_* &= r_1 + a \left( r_* + \frac{r_{in}^2}{r_*} \right), \\
r_* &= r_2 - b \left( \frac{1}{r_*} + \frac{r_*}{r_{ex}^2} \right).
\end{align*}
\] (9)

These equations allow to find the distance between initial tubes which characterize the cylindrical dislocation:

\[
l := r_2 - r_1 = 2ar_* \frac{r_{ex}^2 - r_{in}^2}{r_{ex}^2 - r_*^2},
\] (10)

where expression for \( b \) (8) is used. Afterwards we find the integration constants:

\[
\begin{align*}
a &= \frac{l}{2r_*} \frac{r_{ex}^2 - r_*^2}{r_{in}^2 - r_*^2}, \\
b &= \frac{l}{2r_*} \frac{r_{ex}^2 - r_*^2}{r_{ex}^2 - r_{in}^2}.
\end{align*}
\] (11)

Thus we find the displacement vector field

\[
u(r) := \begin{cases} 
    a \left( r + \frac{r_{in}^2}{r_*} \right) > 0, & r_{in} \leq r < r_*, \\
    -b \left( \frac{1}{r} + \frac{r_*}{r_{ex}^2} \right) < 0, & r_* < r \leq r_{ex}.
\end{cases}
\] (12)

for double wall tube where constants \( a \) and \( b \) are given by Eqs. (11). Qualitative behaviour of this vector field is shown in Fig. 2. Differentiation of this vector field in domains \( r_{in} < r < r_* \), \( r_* < r < r_{ex} \) and its extension to the point \( r_* \) by continuity yields the function

\[
v(r) := \frac{du}{dr} = \begin{cases} 
    a \left( 1 - \frac{r_{in}^2}{r_*^2} \right) > 0, & r_{in} \leq r \leq r_*, \\
    b \left( \frac{1}{r_*} - \frac{1}{r_{ex}^2} \right) > 0, & r_* \leq r \leq r_{ex},
\end{cases}
\] (13)

which is depicted in Fig. 2.

Note that media entirety condition (6) leads to the jump of the displacement vector field at the point \( r_* \):

\[
l := r_2 - r_1 = u_{in}(r_*) - u_{ex}(r_*).
\]

Since vector field \( u \) has discontinuity at the point \( r_* \), the formal derivative of \( u \) contains \( \delta(r - r_*) \). This \( \delta \)-function is thrown away in the geometric theory of defects [14].

Double wall tube with cylindrical dislocation is parameterized by four constants \( r_0, r_1, r_2, r_3 \) or \( r_{in}, r_*, r_{ex}, l \). Formulae (11) define constants \( a, b \) and, consequently, the displacement vector field through the second set of parameters. It follows from definition (1) that there is one-to-one correspondence between two sets of parameters.

Now we calculate the metric induced in double wall tube. By definition, it has the form

\[
g_{\mu\nu}(x) = \frac{\partial y^\rho}{\partial x^\alpha} \frac{\partial y^\sigma}{\partial x^\beta} g_{\alpha\beta}(y),
\] (14)
Figure 2: Qualitative behaviour of the radial component of the displacement vector field for the double wall tube (a). The derivative of the displacement vector field (b).

where $g_{\rho\sigma}(y)$ is the Euclidean metric in cylindrical coordinates. The relation between coordinates before and after defect creation is given by equality (1). Using explicit form of displacement vector field (12) we find the induced metric in the double wall tube

$$ds^2 = (1-v)^2 dr^2 + (r-u)^2 d\varphi^2 + dz^2.$$ (15)

The component $g_{rr} = (1-v)^2$ of this metric is continuous function but its derivative has a jump at $r_*$. The component $g_{\varphi\varphi} = (r-u)^2$ is discontinuous at the point $r = r_*$. The volum element for metric (15) is

$$\sqrt{|g|} = (1-v)(r-u).$$

The right hand side of this relation is positive because both multipliers are positive. The second multiplier $r - u = y > 0$ is positive by construction. The first multiplier is also positive. Indeed, the function $v$ has the maximum at $r = r_*$. At this point, the following inequality holds

$$v(r_*) = a \frac{r_2^2 - r_1^2}{r_*^2} = \frac{r_* - r_1}{r_*} \frac{r_*^2 - r_{in}^2}{r_*^2 + r_{in}^2} < 1,$$

where expression [9] for $a$ is used.

The circumference is a geometric invariant. It is equal to $2\pi(r - u(r))$ for metric (14). When we go from the inner tube to the outer one it has the jump $2\pi l$ where $l$ is the distance between tubes before the dislocation is made. This observation agrees with the continuous model of double wall tube.

1.2 Torsional waves

Here we consider torsional waves in the double wall tube with cylindrical dislocation described in the previous section. We denote the displacement vector field by the new letter $w$ because the letter $u$ was used in the previous section for the displacements corresponding to the defect creation. The total displacement vector field is equal to the sum $u + w$ where $u$ corresponds to the defect creation and $w$ describes oscillations in the double wall tube with cylindrical dislocation. By definition, the displacement vector field $w$ satisfies the wave equation

$$\rho_0 \ddot{w}_i - \mu \nabla^2 w_i - (\lambda + \mu) \nabla_i \nabla_j w^j = 0,$$ (16)
where the covariant derivative $\tilde{\nabla}_i := e^{\mu j} \nabla_\mu$ and Laplace–Beltrami operator $\tilde{\Delta} := g^{\mu \nu} \tilde{\nabla}_\mu \tilde{\nabla}_\nu$ are defined by metric (15) of double wall tube.

This equation is covariant with respect to changing of coordinate systems. It can be solved in cylindrical coordinates $r, \varphi, z$ after the defect creation with metric (15). However it is easier to follow another way. We solve the wave equation in cylindrical coordinates $y, \varphi, z$ where $y$ denotes the old radial coordinate before the defect creation

$$y := r + u,$$

and afterwards impose necessary boundary conditions. It is easier because the metric is Euclidean in the initial coordinate system.

Let us consider torsional waves. In this case only angular component of the displacement vector field differs from zero:

$$\{ w^i \} = \{ w^r = 0, w^\varphi = w^\varphi(t, r), w^z = 0 \}.$$  

From symmetry consideration, the angular component $w^\varphi$ does not depend on $\varphi$ and $z$. For this vector field the $\hat{r}$ and $\hat{z}$ components of Eq.(16) are automatically satisfied. It follows that the dilation for torsional waves is equal to zero

$$\epsilon := \partial_i w^i = 0,$$

and consequently torsional waves take place without media compression.

We look for solution of Eq.(16) in the plain wave form

$$w^\varphi = r e^{i(kz - \omega t)},$$  

where $W(y)$ is the amplitude, $k \in \mathbb{R}$ is the wave vector, and $\omega \in \mathbb{R}$ is the frequency of the wave. Then wave equation (16) in cylindrical coordinates reduces to the Bessel equation

$$r^2 \frac{d^2 U}{dr^2} + r \frac{dU}{dr} + (\kappa^2 r^2 - 1)U = 0,$$  

where

$$\kappa^2 := \frac{\omega^2}{c_t^2} - k^2, \quad c_t^2 := \frac{\mu}{\rho_0}. \tag{19}$$

A general solution of this equation depends on two integration constants. Therefore general solutions for inner and outer tubes are

$$W = \begin{cases} W_{in} = C_1 J_1(\kappa y) + C_2 N_1(\kappa y), & r_0 \leq y \leq r_1; \\ W_{ex} = C_3 J_1(\kappa y) + C_4 N_1(\kappa y), & r_2 \leq y \leq r_3, \end{cases} \tag{20}$$

where $J_1$ is the Bessel function of the first kind and first order, $N_1$ is the Neumann function of the first order (see, i.e. [23]), and $C_{1,2,3,4}$ are integration constants.

To find the integration constants we impose boundary conditions. The boundary surfaces are assumed to be free, i.e. the deformation tensor on the boundary must be zero

$$\frac{dW_{in}}{dr} \bigg|_{r=r_{in}} = 0, \quad \frac{dW_{ex}}{dr} \bigg|_{r=r_{ex}} = 0.$$

Because

$$\frac{dW}{dr} = \frac{dy}{dr} \frac{dW}{dy} = (1 - v) \frac{dW}{dy},$$
and \( v(r_{in}) = v(r_{ex}) = 0 \), these equalities in the initial coordinates take the form

\[
\begin{align*}
C_1 J'_1(z_0) + C_2 N'_1(z_0) &= 0, \\
C_3 J'_1(z_3) + C_4 N'_1(z_3) &= 0,
\end{align*}
\]

where

\[
z := \kappa y,
\]

and prime denotes differentiation with respect to the argument \( z \). These equalities define two integration constants:

\[
C_2 = -k_0 C_1, \quad k_0 := \frac{J'_1(z_0)}{N'_1(z_0)},
\]

\[
C_4 = -k_3 C_1, \quad k_3 := \frac{J'_1(z_3)}{N'_1(z_3)}.
\]

On the gluing surface, we impose two conditions: entirety and equality of stresses,

\[
W_{in}(r_*) = W_{ex}(r_*), \quad \frac{dW_{in}}{dr} \bigg|_{r=r_*} = \frac{dW_{ex}}{dr} \bigg|_{r=r_*}.
\]

As a result we get two equations

\[
\begin{align*}
C_1 \left[ J_1(z_1) - k_0 N_1(z_1) \right] - C_2 \left[ J_1(z_2) - k_3 N_1(z_2) \right] &= 0, \\
C_1 \left[ J'_1(z_1) - k_0 N'_1(z_1) \right] - C_3 \left[ J'_1(z_2) - k_3 N'_1(z_2) \right] &= 0.
\end{align*}
\]

The necessary and sufficient condition for this system to have a nontrivial solution is the equality of its determinant to zero:

\[
\left[ J_1(z_1) - k_0 N_1(z_1) \right] \left[ J'_1(z_2) - k_3 N'_1(z_2) \right] - \\
- \left[ J_1(z_2) - k_3 N_1(z_2) \right] \left[ J'_1(z_1) - k_0 N'_1(z_1) \right] = 0.
\]

For given parameters of the double wall tube \( r_0, r_1, r_2, r_3 \), the obtained relation is the equation for the constant \( \kappa \). Let \( \kappa \) be a root of Eq. (24), then the equality

\[
\omega = c_t \sqrt{k^2 + \kappa^2}.
\]

defines the dispersion relation.

The phase velocity of torsional waves \( v := \omega/k \) is easily found from dispersion relation (25):

\[
v = c_t \sqrt{1 + \frac{\kappa^2}{k^2}}.
\]

The group velocity is also easily found

\[
v_g := \frac{d\omega}{dk} = \frac{c_t^2}{v}.
\]

We see that the phase velocity of torsional waves is always greater than the velocity of transverse waves, and group velocity is smaller. Dispersion relation (25) does depend on double wall parameters through Eq. (24).
2 Conclusion

We found the induced metric in double wall tube with cylindrical dislocation in the framework of the geometrical theory of defect. Though components of this metric are not continuous functions, the three dimensional Einstein equations are well defined ([17]). Afterwards propagation of torsional waves in double wall tube is described. The presence of the cylindrical dislocation inside the double wall tube leads to changing of the dispersion relation.

Double wall tube may be useful as a continuous model of double wall nanotubes.

This work was supported by the Russian Science Foundation (project 14-11-00687) in Steklov Mathematical Institute.

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