

Mechanical Properties of SWNT Within the Framework of the Theory of Ideal Adhesion

Belov Petr A.^{1, *}, Lurie Sergey A.^{1, 2}

¹Department of Non Classical Models of Composites & Structures, Institute of Applied Mechanics RAS, Moscow, Russia

²Department of Mathematical Physics, Computer Center of RAS, Moscow, Russia

Abstract

A model of a two-dimensional defectless medium is formulated as a special case of the general theory of a three-dimensional medium with fields of conserved dislocations, having adhesive properties of a surface that limits the medium. The potential energy in the general theory is the sum of the volume and the superficial integral from the corresponding energy densities. In a limiting case, when the thickness of a shell is equal to zero, the volume portion of potential energy becomes zero. As a result, the potential energy of such an object is defined only by the surface potential energy. A single wall nanotube (SWNT) is examined as an example of such a two-dimensional medium. The problems concerning an SWNT axial deforming as well as the torsional case are examined. The general statement of an axisymmetric problem within the theory of ideal adhesion is formulated. Special cases involving a SWNT deforming axially and in torsion are studied: a case with ideal adhesion, the quasiclassical case, and a case with a large SWNT radius. It is shown that the case with ideal adhesion corresponds to the membrane theory of a cylindrical shell. It is shown that the particular case of the quasiclassical theory of a cylindrical shell is not a logical next step from the general theory when the moduli of ideal adhesion are partially considered and, to a lesser extent, the moduli of purely gradient adhesion. The characteristic feature of all statements is the fact that the mechanical properties of a SWNT are not defined by the “volumetric” moduli but by the adhesive moduli, which have different physical dimensions that coincide with the dimensions of the corresponding stiffness in the classical and nonclassical shells.

Keywords

Gradient Theories of Elasticity, Ideal Adhesion, Gradient Adhesion, Mechanical Properties of SWNT, Nonclassical Moduli

Received: November 24, 2017 / Accepted: December 8, 2017 / Published online: January 16, 2018

© 2017 The Authors. Published by American Institute of Science. This Open Access article is under the CC BY license.

<http://creativecommons.org/licenses/by/4.0/>

1. Introduction

The generalisation of Mindlin’s model described in [1] is investigated. Unlike the “classic” models of Mindlin [2] and Toupin [3], the current model’s generalisation takes into consideration not only the curvatures connected with the gradient of the free distortion in the potential energy volumetric density but also the curvatures associated with the gradient of the restricted distortion as well as the interaction of these two gradients. Another difference arises when considering the generalised model of the surface potential energies (the energy

of adhesion interactions) in the Lagrangian, the surface edge energy, U_s , and the energy of specific points on the surface edge, U_p . Specifically, the Lagrangian of the generalised model can be presented as follows:

$$\begin{aligned}
 L = A - \frac{1}{2} \iiint [& C_{ijmn}^{11} D_j^1 D_{mn}^1 + 2C_{ijmn}^{12} D_j^1 D_{mn}^2 + C_{ijmn}^{22} D_j^2 D_{mn}^2 + \\
 & + C_{ijkml}^{11} D_{jk}^1 D_{ml}^1 + 2C_{ijkml}^{12} D_{jk}^1 D_{ml}^2 + C_{ijkml}^{22} D_{jk}^2 D_{ml}^2] dV - \\
 & - \frac{1}{2} \oint [A_{ijmn}^{11} D_j^1 D_{mn}^1 + 2A_{ijmn}^{12} D_j^1 D_{mn}^2 + A_{ijmn}^{22} D_j^2 D_{mn}^2 + \\
 & + A_{ijkml}^{11} D_{jk}^1 D_{ml}^1 + 2A_{ijkml}^{12} D_{jk}^1 D_{ml}^2 + A_{ijkml}^{22} D_{jk}^2 D_{ml}^2] dF - \\
 & - \sum \oint U_s ds - \sum U_p
 \end{aligned} \tag{1}$$

* Corresponding author

E-mail address: BelovPA@yandex.ru (Belov P. A.)

The kinematic variables of the Lagrangian are the following:

- the continuous portion of the displacement vector R_i ,
- two types of distortions D_{ij}^1 , D_{ij}^2 (restricted and free distortions) and
- two types of curvatures D_{ijk}^1 , D_{ijk}^2 (the gradients of the corresponding distortions).

Between these kinematic variables, there are restrictions defining the kinematic model of such a medium:

$$D_{ij}^1 = R_{i,j} \quad D_{ijk}^1 = R_{i,jk} \quad D_{ij}^2 = D_{ij,k}^2 \quad (2)$$

The moduli tensors C_{ijmn}^{pq} and C_{ijkml}^{pq} define the mechanical properties of the medium volume, and the tensors A_{ijmn}^{pq} and A_{ijkml}^{pq} define the mechanical properties on the medium surface.

This model demonstrates some new qualitative results that are impossible to be obtained in the frames of simpler models. One of such results is studied in this work and is, namely, the opportunity to explain the mechanical properties of a two-dimensional medium, such as SWNT. The Lagrangians in both the classical mechanics of a continuous medium and the well-known gradient models of Mindlin and Toupin contain the potential energy defined only through the volumetric density of the potential energy. Formally, the Lagrangians of these models cannot be applied to the two-dimensional medium. This statement follows from the fact that in these models the potential energy of a zero volume medium is null. In these models, all plate and shell theories are formulated as three-dimensional body models with a small, when compared to others, size in the third direction. Nevertheless, the same substantial mistake exists in the plate/shell theory of these models, i.e., an object with zero volume (due to having zero thickness) will have zero potential energy. One cannot consider the example of a graphene sheet or a SWNT as a volumetric structure having a thickness of approximately on carbon atom diameter as correct [4]. To formulate theories of two-dimensional structures, the Lagrangian is required, which directly contains the surface density of the potential energy. In the same manner as in [6], this work will construct the SWNT theory, and special cases will be investigated.

2. Geometry for SWNT

Coordinates on a cylindrical surface are the following:

$$\begin{cases} x = x \\ y = r \cos \phi \\ z = r \sin \phi \end{cases} \begin{cases} X_i = X_i \\ s_i = \sin \phi Y_i - \cos \phi Z_i \\ n_i = \cos \phi Y_i + \sin \phi Z_i \end{cases} \begin{cases} X_i = X_i \\ Y_i = \sin \phi s_i + \cos \phi n_i \\ Z_i = -\cos \phi s_i + \sin \phi n_i \end{cases} \quad (3)$$

The coordinates are defined as the following: x, y, z - the Cartesian coordinates, x, ϕ, r - cylindrical coordinates, X_i - ort of an axial coordinate, s_i - ort of distinct coordinate, n_i - ort of a normal to a cylindrical surface.

Kronecker's "flat" tensor is the following:

$$\delta_{ij}^* = (\delta_{ij} - n_i n_j) = X_i X_j + s_i s_j \quad (4)$$

The gradient on a cylindrical surface is the following:

$$\begin{aligned} \frac{\partial(\dots)}{\partial x_j} &= \frac{\partial(\dots)}{\partial y_k} \frac{\partial y_k}{\partial x_j} = \frac{\partial(\dots)}{\partial x} \frac{\partial x}{\partial x_j} + \frac{\partial(\dots)}{\partial r} \frac{\partial r}{\partial x_j} + \frac{\partial(\dots)}{\partial \phi} \frac{\partial \phi}{\partial x_j} = \\ &= \frac{\partial(\dots)}{\partial x} X_j + \frac{\partial(\dots)}{\partial \phi} \frac{1}{r} [\sin \phi Y_j - \cos \phi Z_j] = \frac{\partial(\dots)}{\partial x} X_j + \frac{\partial(\dots)}{\partial \phi} \frac{1}{r} s_j \end{aligned} \quad (5)$$

The derivatives of the orts of a cylindrical surface is the following:

$$s_{i,j} = \frac{1}{r} n_i s_j \quad n_{i,j} = -\frac{1}{r} s_i s_j \quad (6)$$

The displacement vector is the following:

$$R_i = r_i + W n_i = U(x, \phi) X_i + V(x, \phi) s_i + W(x, \phi) n_i \quad (7)$$

The restricted distortion (displacement derivatives) tensor is the following:

$$\begin{aligned} R_{i,j} &= \left[\frac{\partial U}{\partial x} X_i + \frac{\partial V}{\partial x} s_i + \frac{\partial W}{\partial x} n_i \right] X_j + \\ &+ \left[\frac{\partial U}{\partial \phi} X_i + \left(\frac{\partial V}{\partial \phi} - W \right) s_i + \left(V + \frac{\partial W}{\partial \phi} \right) n_i \right] \frac{1}{r} s_j \end{aligned} \quad (8)$$

3. Variational Statement of the SWNT Theory

In the case of the Lagrangian (1), if the medium volume is null, the Lagrangian becomes a specific, nontrivial form:

$$\begin{aligned} L &= A - \frac{1}{2} \iint [A_{ijmn}^{11} D_{ij}^1 D_{mn}^1 + 2A_{ijmn}^{12} D_{ij}^1 D_{mn}^2 + A_{ijmn}^{22} D_{ij}^2 D_{mn}^2 + \\ &+ A_{ijkml}^{11} D_{ijk}^1 D_{mnl}^1 + 2A_{ijkml}^{12} D_{ijk}^1 D_{mnl}^2 + A_{ijkml}^{22} D_{ijk}^2 D_{mnl}^2] dF \end{aligned} \quad (9)$$

If we consider a SWNT as an ideal two-dimensional structure, we should put aside all terms containing the free distortion tensor D_{ij}^2 from expression (9) because this tensor determines the defectness of the medium that is being studied. The Lagrangian becomes the following:

$$L = A - \frac{1}{2} \oint [A_{ijmn}^{11} D_{ij}^1 D_{mn}^1 + A_{ijknml}^{11} D_{ijk}^1 D_{mnl}^1] dF \quad (10)$$

Additionally, as a SWNT is a two-dimensional structure, the surface density of the potential energy should not depend on the normal derivatives of the displacements. Associated with this fact, we should require that the tensors of the adhesive moduli have the following properties:

$$\begin{aligned} A_{ijmn}^{11} n_j &= A_{ijmn}^{11} n_n = 0 \\ A_{ijknml}^{11} n_j &= A_{ijknml}^{11} n_k = A_{ijknml}^{11} n_n = A_{ijknml}^{11} n_l = 0 \end{aligned} \quad (11)$$

For the formulation of a mathematical theory concerning momentless cylindrical shells, we use a classic method of allocation by slowly changing (membrane) state. For this purpose, we will neglect the potential energy curvatures (second item in the superficial integral in (10)) in comparison with the potential energy of the deformation (first item in the superficial integral in (10)).

To simplify the task, let us accept the idea that the mechanical properties are isotropic on the SWNT surface. The result of (11) and (10) gives the following adhesive tensors, which are less complex compared with (1):

$$A_{ijmn}^{11} = a_1^{11} \delta_{ij}^* \delta_{mn}^* + a_2^{11} (\delta_{im}^* \delta_{jn}^* + \delta_{in}^* \delta_{jm}^*) + a_6^{11} n_i n_m \delta_{jn}^* \quad (12)$$

By expanding the structure of the potential energy for an axisymmetric problem, the potential energy becomes the following:

$$\begin{aligned} U_F &= \frac{1}{2} [a_1^{11} (U' - W/r)(U' - W/r) + a_6^{11} (W'W' + VV/r^2) + \\ &+ a_2^{11} (2U'U' + V'V' + VV/r^2 + W'W' + 2WW/r^2)] \end{aligned} \quad (13)$$

We can define the force factors using Green's formulae:

$$\sigma_{ij} = \frac{\partial U_F}{\partial R_{i,j}} = A_{ijmn} R_{m,n} \quad (14)$$

The corresponding variation equation follows from Lagrange's principle.

The variation equation in the force factors is the following:

$$\begin{aligned} \delta L &= 2\pi r \int_0^l (\sigma_{ij,j} + P_i^F) \delta R_i dx + \\ &+ 2\pi r (P_i - \sigma_{ij} X_j) \delta R_i \Big|_{x=0}^{x=l} = 0 \end{aligned} \quad (15)$$

The variation equation in the displacement is the following:

$$\begin{aligned} \delta L &= 2\pi r \int_0^l \{ [(a_1^{11} + 2a_2^{11})U'' - a_1^{11}W'/r + P_x^F] \delta U + \\ &+ [a_2^{11}V'' - (a_2^{11} + a_6^{11})V/r^2 + P_\phi^F] \delta V + \\ &+ [a_1^{11}U'/r + (a_2^{11} + a_6^{11})W'' - (a_1^{11} + 2a_2^{11})W/r^2 + P_r^F] \delta W \} dx + \\ &+ 2\pi r \{ [P_x^C - (a_1^{11} + 2a_2^{11})U' + a_1^{11}W/r] \delta U + \\ &+ [P_\phi^C - a_2^{11}V'] \delta V + \\ &+ [P_r^C - (a_2^{11} + a_6^{11})W'] \delta W \} \Big|_{x=0}^{x=l} = 0 \end{aligned} \quad (16)$$

The system of equilibrium equations becomes the following:

$$\begin{cases} (a_1^{11} + 2a_2^{11})U'' - a_1^{11}W'/r + P_x^F = 0 \\ a_2^{11}V'' - (a_2^{11} + a_6^{11})V/r^2 + P_\phi^F = 0 \\ a_1^{11}U'/r + (a_2^{11} + a_6^{11})W'' - (a_1^{11} + 2a_2^{11})W/r^2 + P_r^F = 0 \end{cases} \quad (17)$$

Special attention should be paid such that the torsion in the new theory is separated from the tension/compression. It is interesting to consider these cases separately. Such case will allow us to carry out comparison using the classical theory of cylindrical shells.

4. The Mechanical Properties of a SWNT While Deforming Axial

Let us assume that torsion is absent. Then, displacement V is equal to zero, and the system of equilibrium equations becomes the following:

$$\begin{cases} (a_1^{11} + 2a_2^{11})U'' - a_1^{11}W'/r + P_x^F = 0 \\ a_1^{11}U'/r + (a_2^{11} + a_6^{11})W'' - (a_1^{11} + 2a_2^{11})W/r^2 + P_r^F = 0 \end{cases} \quad (18)$$

The first equilibrium equation has a quadrature:

$$\begin{cases} U' = \frac{a_1^{11}}{(a_1^{11} + 2a_2^{11})} W/r + \frac{1}{(a_1^{11} + 2a_2^{11})} N(x) \\ (a_2^{11} + a_6^{11})W'' - 4 \frac{a_2^{11}(a_1^{11} + a_2^{11})}{(a_1^{11} + 2a_2^{11})} W/r^2 + P_r^F + \frac{a_1^{11}}{(a_1^{11} + 2a_2^{11})} N_x^F(x)/r = 0 \end{cases} \quad (19)$$

Here $N_x^F(x)$ is the stretching force. Using the second equilibrium equation, it is possible to determine the second quadrature:

$$\begin{cases} U = U_0 + \frac{a_1^{11}(a_2^{11} + a_6^{11})r}{4a_2^{11}(a_1^{11} + a_2^{11})} W' + \\ + \int_0^x \left[\frac{a_1^{11}}{4a_2^{11}(a_1^{11} + a_2^{11})} r P_r^F + \frac{a_1^{11} a_1 + 4a_2^{11}(a_1^{11} + a_2^{11})}{4a_2^{11}(a_1^{11} + a_2^{11})(a_1^{11} + 2a_2^{11})} N_x^F(x) \right] dx \\ W'' - \frac{4a_2^{11}(a_1^{11} + a_2^{11})}{(a_2^{11} + a_6^{11})(a_1^{11} + 2a_2^{11})r^2} W = - \frac{1}{(a_2^{11} + a_6^{11})} [P_r^F + \frac{a_1^{11}}{(a_1^{11} + 2a_2^{11})} N_x^F(x)/r] \end{cases} \quad (20)$$

The boundary problem will also be transformed in terms of deflections:

$$2\pi r \{ [P_x^C - N_x^F(x)] \delta U + [P_r^C - (a_2^{11} + a_6^{11}) W'] \delta W \} \Big|_{x=0}^{x=l} = 0 \quad (21)$$

Therefore, the mathematical theory of momentless cylindrical shells in the framework of ideal adhesion theory is formulated. This theory is applicable to both nanotubes and to macroshells provided that their thickness is equal to zero (the potential energy is defined exclusively by the surface density of the potential energy as the shell's material thickness/volume are equal to zero by definition). We will pay attention that the boundary problem in terms of the deflection contains only one coupled boundary condition: deflections W or Saint-Venant's cutting force $(a_2^{11} + a_6^{11})W'$ are defined at end edges of the nanotube.

Therefore, the adhesive modulus $(a_2^{11} + a_6^{11})$ has physical sense of rigidity on the shift and has the same physical dimension (Pa*m or J/sq.m). As in the mathematical theory of nanoplates/graphene sheets [6], this rigidity is a multiplier of a slowly changing second order item in graphene theory [9].

With sufficient confidence, it is possible to assure that in the theory of nanotubes the classic balance operator has the additional item. If we reject for a moment a membrane hypothesis, we can subtract the fourth derivative of the deflection from the deflection equation, and we will obtain the following:

$$-DW'''' + (a_2^{11} + a_6^{11})W'' - \frac{4a_2^{11}(a_1^{11} + a_2^{11})}{(a_1^{11} + 2a_2^{11})r^2} W = -[P_r^F + \frac{a_1^{11}}{(a_1^{11} + 2a_2^{11})} N_x^F(x) / r] \quad (22)$$

where D is the cylindrical stiffness of a nanotube, which, for shells of zero thickness, has to be defined by the components of the sixth rank adhesive moduli tensor according to (10-11).

Neglecting the item in equation (22), which contains the second derivative of the deflection, we will obtain the "classic" equation for a cylindrical shell (with reservations concerning other physical senses of stiffness).

As the radius of a tube goes to infinity, i.e., in case of a tube's degeneration in a graphene sheet, we will obtain equation for 2D-structures and the theory of a graphene sheet as in [6].

We will give special attention that, unlike the theory of tension/compression of thin-walled shells, in the theory of tension/compression in nanotubes there is no fundamental decision with regards to constant axial deformation. The edge effect (with characteristic length l_*) is defined by the relation of the adhesive moduli with an identical dimension:

$$l_* = r \sqrt{\frac{(a_2^{11} + a_6^{11})(a_1^{11} + 2a_2^{11})}{4a_2^{11}(a_1^{11} + a_2^{11})}} \quad (23)$$

This is truly an edge effect not a multiscale effect because it is defined by the relative size of a body not the relative moduli of different dimensions.

At the rather large nanotube radii and when the third term in (22) can be neglected in comparison with the second term, the tension/compression theory of nanotubes degenerates to the classical theory of thin-walled shells (while maintaining a physical sense of the moduli that appears in the equation). Therefore, we have two ratios, $Gh = (a_2^{11} + a_6^{11})$ and l_* (23), for three connecting adhesive moduli $a_1^{11}, a_2^{11}, a_6^{11}$ that must experimental defined. If the third combination of the adhesive moduli can be formulated in the equilibrium equations, there is an opportunity to formulate experimental tests to directly define all three moduli.

5. The Mechanical Properties of SWNT While in Torsion

Given the definition of the potential energy defining the SWNT statement (13) and the torsional constraints $U = 0, W = 0$, the variational equation becomes the following:

$$\delta L = 2\pi r \int_0^l [a_2^{11} V'' - (a_2^{11} + a_6^{11}) V / r^2 + P_\phi^F] \delta V dx + 2\pi r [P_\phi^C - a_2^{11} V'] \delta V \Big|_{x=0}^{x=l} = 0 \quad (24)$$

The boundary problem is reduced to two boundary conditions: either the angle of rotation V / r is defined or the torque $a_2^{11} V'$ is defined. The analogue of Bredt's stiffness a_2^{11} can be defined from the experimental torsional scales where instead of a thread a nanotube is used.

We will make certain that, unlike in the theory of the torsion of thin-walled cores, in the theory of torsion of nanotubes there is no fundamental decision to define a constant twisting angle. The edge effect (which is determined by the characteristic length) is defined by the relationship between adhesive analogues of torsional a_2^{11} and the shift $(a_2^{11} + a_6^{11})$ stiffnesses:

$$l_0 = r \sqrt{\frac{a_2^{11}}{(a_2^{11} + a_6^{11})}} \quad (25)$$

This is truly an edge effect not a multiscale effect because it is defined by the relative sizes of a body not the relative

moduli of different dimensions.

At the rather large nanotube radii and when the second item in (24) can be neglected in comparison with the first term, the theory of nanotube torsion degenerates to the classical theory of thin-walled cores (while maintaining a physical sense of the moduli that appears in the equation).

6. Conclusions

The applied theories for an SWNT axial deforming and a SWNT torsion formulated in this work offer possibilities to study the mechanical properties of 2D media and to set and solve test problems. The solutions developed from this work can be tested experimentally. Specifically, during the axial deforming of a SWNT, it possible to reduce the SWNT's mechanical properties to the two non-classical adhesive moduli a_1^{11} and a_6^{11} and correspondingly, the torsional deformation problem can be reduced to one modulus: a_2^{11} .

The formulated membrane theory of nanotubes does not describe the multiscale effects [7, 10, 11]. Nevertheless, within this theory, there are nonclassical edge effects that are absent in the classical theory of thin-walled cores. Characteristic lengths of these edge effects are proportional to the radius of a tube and the dimensionless relationship of the adhesive moduli that are defined in the ratios in (23) and (25).

We should focus our attention to the fact that the model formulated in this work can be generalised to a general SWNT theory if we reject the membrane hypothesis and transform from a Lagrangian with potential energy as defined in (13) to a Lagrangian as defined in (11). This generalization was carried out in works [6, 8].

Acknowledgements

This work was carried out within the framework of the state program at the Institute of Applied Mechanics of RAS and was supported particularly by the Russian Foundation of Basic Research grants 15-01-03649-a.

References

- [1] Belov Petr A. «The theory of continuum with conserved dislocations: generalisation of Mindlin theory», «Composites and nanostructures», 2011, Volume 3, №1, pp. 24-38.
- [2] Mindlin R. D. «Micro-structure in linear elasticity», «Archive of Rational Mechanics and Analysis», 1964, №1, p. 51-78.
- [3] Toupin R. A. «Elastic materials with couple-stresses», «Archive of Rational Mechanics and Analysis», 1964, №2, p. 85-112.
- [4] Geim A. K., Novoselov K. S., Jiang D., Schedin F., Booth T. J., Khotkevich V. V., Morozov S. V. «Two-dimensional atomic crystals», PNAS 102, 10451 (2005) DOI:10.1073/pnas.0502848102
- [5] Belov Petr A., Lurie S. A. «The theory of ideal adhesion interactions», "The mechanics of composite materials and designs", 2007, Volume 14, №3, pp. 519-536.
- [6] Belov Petr A. «Mechanical properties of graphene within the framework of gradient theory of adhesion», "Journal of Civil Engineering and Architecture", 2014, V. 8, №6, page 693-698.
- [7] Belov P. A., Lurie S. A., H. Altenbach Classification of gradient adhesion theories across length scale, Springer International Publishing Switzerland 2016, H. Altenbach and S. Forest (eds.), In book: Generalized Continua as Models for Classical and Advanced Materials, Advanced Structured Materials 42, ISBN 978-3-319-31721-2.
- [8] Belov PA, Lurie SA Mathematical theory of damaged media. Gradient theory of elasticity. Formulations. Hierarchy. Comparative analysis. 2014, Palmarium Academic Publishing, Germany, 336p, ISBN 978-3-639-73761-5
- [9] Belov P. A., Nelyub V. A., The Timoshenko theory of plates with adhesive properties of face surfaces, Polymer Science, Series D, 2015, V8, №4, p. 307-309.
- [10] Sergey A. Lurie, P. A. Belov, K. D. Kharchenko, The theory of media with defect fields and models of deformation of functional layers in isotropic materials, Nanomechanics Science and Technology: An International Journal, 2015, V.6, №1, p. 1–16.
- [11] Sergey A. Lurie, P. A. Belov, Dmitriy B. Volkov-Bogorodsky, E. D. Lykosova, Do nanosized rods have abnormal mechanical properties? Nanomechanics Science and Technology: An International Journal, 2016, V.7, №4, p.1–35.