A NOTE ON THE EQUILIBRIUM SHAPES OF CARBON NANOTUBES SUBJECTED TO HYDROSTATIC PRESSURE

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ABSTRACT. This note deals with the problem for determination of possible equilibrium shapes of carbon nanotubes subjected to hydrostatic pressure. There exists a large amount of literature in this field but it is assumed therein that the deformed nanotube is a cylindrical surface and only the shape of the tube directrix changes. In this study, using the continuum approach to the analysis of carbon nanostructures suggested by Tu and Ou-Yang, we find that non-cylindrical equilibrium shapes of carbon nanotubes under hydrostatic pressure also exist. Several examples of such shapes that are axially symmetric unduloid-like surfaces are determined.

Key words: carbon nanotubes, hydrostatic pressure, continuum approach, equilibrium shapes, unduloid.

1. Introduction

Carbon nanotubes are carbon molecules in the shape of hollow cylindrical fibers of nanometer-size diameter and length-to-diameter ratio of up to $10^7 : 1$. Carbon nanotubes exhibit extraordinary strength, unique electrical properties, and are efficient conductors of heat. For this reason, carbon nanotubes have many practical applications in electronics, optics and other fields of material science.

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Two approaches for computation of the shapes of these structures exist. Within the first one, often referred to as molecular dynamic (MD) simulations, the carbon nanotube is considered as a multibody system in which the interaction between atoms is modelled through certain empirical interatomic potentials. In 1988 Tersoff [1] suggested a general approach for derivation of such potentials and applied it to silicon. In 1990, Brenner [2] adapted and modified Tersoff’s results and suggested an interatomic potential for carbon atomic bonds that is in use up to now. Another potential of such kind was presented in 1992 by Lenosky et al. [3].

The second approach, often referred to as a continuum approach, was introduced by Yakobson et al. [4] in 1996, and consists in application of a certain classical theory of isotropic thin elastic shells for explanation of the mechanical properties and exploration of the deformed shapes of these carbon molecules. The advantage of such an approach, in comparison with the ones based directly on the interatomic interactions, is that the continuum mechanics models are amenable to analytical calculations and allow efficient numeric simulations. Since the pioneering work [4], the use of continuum mechanics concepts in nanostructure mechanics has become common practice although, as noted therein, “its relevance for a covalent-bonded system of only a few atoms in diameter is far from obvious”. The easiest way of introducing a continuum model of the regarded atomistic systems is to adopt a standard continuum theory (e.g., some of the well-known shell theories) and to adjust the material parameters to the data available by experimental observations or MD simulations. The more sophisticated attempts at deriving continuum theories for carbon nanotubes incorporate the specific atomic lattice structure and are based on the aforementioned interatomic potentials. The essential idea behind this kind of theories is to express the deformation of the atomic lattice in terms of the geometric quantities that characterize the deformation of the continuum using an appropriate continuum limit [5, 6] or kinematic assumptions such as the Cauchy-Born rule or its modifications [7, 8].

There exists a vast amount of papers concerning the behaviour of carbon nanostructures subjected to various excitations. In what concerns carbon nanotubes subjected to hydrostatic pressure, only their cylindrical equilibrium shapes are regarded in the majority of the works on this topic (see, e.g. [9] and references therein). It was established [9] that the differential equations describing the cylindrical equilibrium shapes of carbon nanotubes are the same as the equations governing the equilibrium shapes of elastic rings under pressure. Thus, it is found that if the dimensionless pressure is less than 3, then only the circular shape of the carbon nanotubes exists. Non-circular shapes
exists for higher pressure only.

Axisymmetric shapes of carbon nanotubes are much rarely reported in the literature. Xie et al [10] present observations of such shapes, but as a result of fluctuation of the tube growth conditions – pressure, temperature and chemical composition of the vapour atmosphere around the tube.

In this contribution, axisymmetric equilibrium shapes of carbon nanotubes subjected to hydrostatic pressure are determined applying the continuum approach suggested in [6]. The respective differential equations and boundary conditions are solved numerically and several examples of such shapes are presented. It is found that axisymmetric equilibrium shapes of carbon nanotubes exist even for pressure less than 3, unlike the case of cylindrical equilibrium shapes.

2. Differential equations and boundary conditions

In this work, we follow to continuum approach developed by Tu and Ou-Yang in 2008 [6] which is based on a revised version of the potential suggested by Lenosky et al [3]. Within this approach, the tube is regarded as a two-dimensional surface $S$ embedded in the three-dimensional Euclidean space $\mathbb{R}^3$. This surface is assumed to exhibit purely elastic deformation consisting of bending, described by its mean $H$ and Gaussian $K$ curvatures, and stretching, described by the linear $J$ and quadratic $Q$ invariants of the in-plane strain tensor of the surface $S$. Its equilibrium shapes are determined by the extrema of the deformation energy functional

$$F_c = 2k_c \int_S H^2 dA - k_G \int_S K dA + 2k_d \int_S J^2 dA - \bar{k} \int_S Q dA$$

(2.1)

where, $k_c$ and $k_G$ are two material constants associated with the bending rigidity, and $k_d$ and $\bar{k}$ are other two material constants associated with the in-plane stretching rigidity of this surface.

Let us recall the experimental observations implying that carbon nanotubes are more pliable to bending than to stretching. For this reason, a widely used approximation inherent to the continuum approach is to neglect the stretching energy in comparison with the bending one and to consider the tube as inextensible. Then, neglecting the last two terms in (2.1) and substituting them with an inextensibility constraint we arrive at a functional of form

$$F_c = 2k_c \int_S H^2 dA - k_G \int_S K dA + \lambda \int_S dA + p \int_V dV,$$

(2.2)

where $\lambda$ is a Lagrangian multiplier corresponding to the constraint of fixed
area of the surface $S$, and the last term is the work done by the pressure $p$ in the deformation of the volume $V$ whose boundary is $S$. Thus, given a pressure $p$, the equilibrium shapes of the surface $S$ are determined by the extrema of the functional (2.2).

This functional is a basic tool for analysis of the equilibrium shapes of lipid bilayer membranes in the Helfrich theory [11]. The corresponding Euler-Lagrange equation reads

\[ \Delta H + (H^2 - K)H - \sigma H + q = 0, \quad \sigma = \frac{\lambda}{k_c}, \quad q = \frac{p}{k_c}, \]

where $\Delta$ is the Laplace-Beltrami operator of the surface $S$ (see [12]).

If the surface $S$ is axisymmetric, it is completely determined by its profile curve (contour). Therefore, we seek plane curves which, being rotated about a line, form surfaces whose mean curvatures satisfy the shape equation (2.3). Let $x = x(s), \ z = z(s)$ be the parametric equations of the contour in the Cartesian frame ($x, z$), where $s$ denotes the contour arclength and $z$ is the axis of symmetry. Let $\psi$ stands for the angle between the tangent vector of the contour and the $x$-axis. Then,

\[ 2H = \frac{\sin \psi}{x} + \frac{d\psi}{ds}, \quad K = \frac{\sin \psi}{x} \frac{d^2\psi}{ds^2}, \]

and the shape equation can be written in the form (see [13])

\[ \frac{d^3\psi}{ds^3} = -\frac{2 \cos \psi}{x} \frac{d^2\psi}{ds^2} - \frac{1}{2} \left( \frac{d\psi}{ds} \right)^3 + \frac{3 \sin \psi}{2x} \left( \frac{d\psi}{ds} \right)^2 \]

\[ + \frac{2\sigma x^2 + 2 - 3\sin^2 \psi}{2x} \frac{d\psi}{ds} + \frac{2\sigma x^2 - 2 + \sin^2 \psi}{2x^3} \sin \psi + 2q. \]

Here, the unknown functions are $\psi(s)$ and $x(s)$, which are also related by the classic geometric formula

\[ \frac{dx}{ds} = \cos \psi. \]

Thus, equations (2.4)–(2.5) constitute a closed system for the unknowns $\psi(s)$ and $x(s)$. Once $\psi(s)$ is determined, then $z(s)$ can be obtained by $dz/ds = \sin \psi$.

In this study we are seeking surfaces of finite length that are symmetric with respect to the $z$-axis. Three boundary conditions hold [6] at each free edge (a circle corresponding to $s = s_0$) of such a surface, and in the case $\psi(s_0) = -\pi/2$, they reduce to

\[ \left. \frac{d\psi}{ds} \right|_{s=s_0} - \left( 1 - \frac{k_G}{k_c} \right) \frac{1}{x(s_0)} = 0, \quad \frac{k_G}{2k_c} \left( 2 - \frac{k_G}{k_c} \right) \frac{1}{x^2(s_0)} + \sigma = 0. \]
A Note on the Equilibrium Shapes of Carbon Nanotubes . . .

Fig. 1. Profile curves and the corresponding shapes of carbon nanotube with length $L = 1$ and parameters: (a) $q = 2.02$, $k_G/k_c = 0.75$; (b) $q = 30.33$, $k_G/k_c = -1.38$.

Fig. 2. Profile curve and the corresponding shape of a carbon nanotube with parameters $L = 1.56$, $q = 528.18$, $k_G/k_c = -2$.

Solving numerically the system (2.4)–(2.5) and these boundary conditions we are now able to obtain equilibrium shapes of carbon nanotubes under pressure.

3. Results and discussion

First, it is found that axisymmetrically deformed tube shapes exist even for $q < q_c = 3$, a typical example being the contour in Fig. 1a, corresponding to a pressure $q = 2.02$. However, the maximal value of the deflection of the tube from the circular cylindrical shape is less than 1% of the radius of the cylinder and therefore, the deformation of the tube is unnoticeable. For higher pressures, the tube bending is more pronounced as is seen in Fig. 1b. Finally, peculiar equilibrium shapes are obtained at very high pressures, a typical example being shown in Fig. 2.

REFERENCES


