The pseudospherical reduction of an uniaxial deformation of the Carbon nanotubes

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Abstract

This paper is focused on the single-walled carbon nanotubes with different radius and chirality (armchair $(n,\ n)$, chiral $(2n,\ n)$, and zigzag $(n,\ 0)$), and perfect circular cross section, subjected to tensile loading. The aim is to determine a parametrical representation for a class of constitutive laws for which the motion equations attached to a material system can be associated to a pseudospherical surface (with negative Gaussian curvature K). A genetic algorithm is performed to study some inverse problems associated to some experimental results.

Mathematics Subject Classification: 37N15, 14Rxx.
Key words: Carbon nanotubes, pseudospherical surface, Gaussian curvature, constitutive law, uniaxial deformation.

1 Introduction

The carbon nanotubes as a quasi-one-dimensional structures were discovered by Iijima [1], Iijima and Ichihashi [2]. The carbon nanotube is one of the most promising building blocks for future development of functional nanostructures (Srivastava, Menon and Cho [3], Gao, Cagin and Goddard [4]). The single-walled carbon nanotubes can be regarded as a rolled-up graphite sheet in cylindrical form. Thess and co-workers [5] produced crystalline ropes of metallic carbon nanotubes with 100–500 single-walled carbon nanotubes bundled into a two-dimensional triangular lattice. These ropes are expected to have remarkable mechanical, electronic and magnetic properties. The nanotube is a cylindrical molecule composed of carbon atoms, with open or closed ends. A typical section of a single-walled carbon nanotube is illustrated in Fig. 1.1, each node being a carbon atom and lines the chemical bonds (Ruoff *et al.* [6]).

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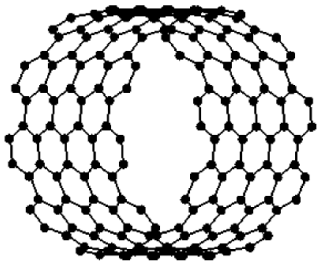

Fig. 1.1. A section through a carbon nanotube (zigzag)
viewed from the side (after Ruoff *et al.* [6]).

In this paper we try to find a class of constitutive laws by applying the pseudospherical reduction method for the carbon nanotubes mechanical problem. By this reduction, the motion equations are associated to a pseudospherical surface Σ, with negative Gaussian curvature K (Rogers and Schief, [7], [8], Chiroiu *et al.* [9]). If the ratio K/d^4, where d is the distance from the origin to the tangent plane at an arbitrary point, is constant, then we obtain a Ţiţeica surface (Ţiţeica [10], [11], Teodorescu *et al.* [12], [13]). The Ţiţeica surfaces are invariants under the group of centroaffine transformations, being analogues of spheres in affine differential geometry. At present, only a few achievements have been made to determine the parametrical representation of a class of constitutive laws for which the motion equations attached to the material system can be associated to a pseudospherical surface. We consider that this novel approach may improve the estimation of structurally sensitive carbon nanotubes properties. The constitutive laws for single-walled carbon nanotubes are determined by applying the pseudospherical reduction method and a genetic algorithm.

2 The pseudospherical reduction of the problem

Consider the 1D problem of uniaxial deformation of a single wall carbon nanotube modelled by a nonhomogeneous bar. We present in this section the pseudospherical reduction of the problem in the spirit of Rogers and Schief [7], [8]. The governing equations in a Lagrangian system of coordinates (X,t) read

$$\varepsilon_t = v_X, \quad \rho_0 v_t = \sigma_X. \tag{2.1}$$

The general constitutive law is given by

$$\sigma = \sigma(\varepsilon.X). \tag{2.2}$$

Here, σ and ρ are the uniaxial stress and the density of the material, respectively $\varepsilon = \frac{\rho_0}{\rho} - 1$ is the strain, ρ_0 is the density of the material in the underformed state, and $v(X,t)$ is the material velocity. In terms of the Eulerian coordinates $x = x(X,t)$, we have

$$\mathrm{d}x = (\varepsilon + 1)\mathrm{d}X = v\mathrm{d}t, \tag{2.3}$$

so that

$$\rho_0 \mathrm{d}X = \rho \mathrm{d}x - \rho v \mathrm{d}t. \tag{2.4}$$

In (2.4), X corresponds to the particle function ψ of the Martin formulation. The independent variables are chosen to be σ and ψ, and we suppose $\rho_0 = 1$. In this case we obtain the Monge–Ampère equation

$$\xi_{\sigma\sigma}\xi_{\psi\psi} - \xi_{\sigma\psi}^2 = \varepsilon_\sigma, \tag{2.5}$$

where

$$\begin{gathered} t = \xi_\sigma, \quad v = \xi_\psi, \\ \mathrm{d}x = \xi_\psi \xi_{\sigma\sigma} + (\xi_\psi \xi_{\sigma\psi} + \varepsilon)\mathrm{d}\psi, \\ 0 < |\xi_{\sigma\sigma}\varepsilon| < \infty. \end{gathered} \tag{2.6}$$

If a solution $\xi(\sigma, \psi)$ of this equation is specified, then the particle trajectories are calculated from

$$x = \int [\xi_\psi \xi_{\sigma\sigma} + (\xi_\psi \xi_{\sigma\psi} + \varepsilon)\mathrm{d}\psi], \quad t = \xi_p, \tag{2.7}$$

in terms of σ, for $\psi = \text{const}$. By solving (2.7), the solution $\sigma(\psi, t)$ is obtained, and the original solution of (2.1)–(2.2) is parametrically determined in terms of the Lagrangian variables

$$x = x(\psi, t), \quad v = v(\psi, t), \quad \sigma = \sigma(\psi, t). \tag{2.8}$$

Rogers and Schief (1997) made the geometric connection to this problem. To show this, let us consider a surface Σ in R^3 written Monge parametrization

$$r = xe_1 + ye_2 + z(x, y)e_3, \tag{2.9}$$

where $r = r(x, y, z)$ is the position vector of a point P on the surface

The first and second fundamental forms are defined as

$$\begin{aligned} I &= E\mathrm{d}x^2 + 2F\mathrm{d}x\mathrm{d}y + G\mathrm{d}y^2 \\ &= (1 + z_x^2)\mathrm{d}x^2 + 2z_x z_y \mathrm{d}x\mathrm{d}y + (1 + z_y^2)\mathrm{d}y^2, \\ II &= e\mathrm{d}x^2 + 2f\mathrm{d}x\mathrm{d}y + g\mathrm{d}y^2 \\ &= \frac{1}{\sqrt{1+z_x^2+z_y^2}}(z_{xx}\mathrm{d}x^2 + 2z_{xy}\mathrm{d}x\mathrm{d}y + z_{yy}\mathrm{d}y^2). \end{aligned} \tag{2.10}$$

The Gaussian curvature of Σ is

$$\mathrm{K} = \frac{eg - f^2}{EG - F^2} = -\frac{z_{xx}z_{yy} - z_{xy}^2}{(1 + z_x^2 + z_y^2)^2}. \tag{2.11}$$

If Σ is a hyperbolic surface, then the total curvature is negative and the asymptotic lines on Σ may be taken as parametric curves. Let us introduce the same independent variables as before, i.e.

$$\sigma = z_x, \quad \psi = z_y, \tag{2.12}$$

and the dependent variables

$$\xi_\sigma = x, \quad \xi_\psi = y. \tag{2.13}$$

Therefore, we have

$$\xi_{\sigma\sigma} = \frac{z_{yy}}{z_{xx}z_{yy} - z_{xy}^2}, \quad \xi_{\psi\psi} = \frac{z_{xx}}{z_{xx}z_{yy} - z_{xy}^2}, \quad \xi_{\sigma\psi} = \frac{z_{xy}}{z_{xx}z_{yy} - z_{xy}^2}. \tag{2.14}$$

The Gaussian curvature (2.10) yields

$$K = \frac{1}{(1+\sigma^2+\psi^2)^2(\xi_{\sigma\sigma}\xi_{\psi\psi} - \xi_{\sigma\psi}^2)}, \tag{2.15}$$

and may be set into correspondence with Martin's Monge–Ampère equation (2.5) by

$$\varepsilon_\sigma = \frac{1}{\mathrm{K}(1+\sigma^2+\psi^2)^2}, \tag{2.16}$$

and

$$\mathrm{K} = \frac{A^2}{(1+\sigma^2+X^2)^2}. \tag{2.17}$$

where $A^2 = \frac{\partial\sigma}{\partial\varepsilon|_X}$, with A the Lagrangian wave velocity. The surface Σ is restricted to be pseudospherical, that is

$$K = -\frac{1}{a^2}, \quad a = \text{const.} \tag{2.18}$$

In this case the relation (2.17) gives

$$\frac{\partial^2\sigma}{\partial\varepsilon^2|_X} = \frac{2}{a^2}(1+\sigma^2+X^2)\sigma\frac{\partial\sigma}{\partial\varepsilon}|_X > 0, \quad \sigma > 0. \tag{2.19}$$

Integrating (2.19), we have

$$\varepsilon = \frac{a^2}{2(1+X^2)^{3/2}}\left[\arctan\left(\frac{\sigma}{1+X^2}\right) + \frac{\sigma\sqrt{1+X^2}}{1+\sigma^2+X^2}\right] + \alpha(X), \tag{2.20}$$

with $\alpha(X)$arbitrary. For $\sigma|_{\varepsilon=0} = 0$ it results $\alpha(X)$=0.

The relation (2.20) represents a class of constitutive laws for which the equations (2.1) are associated to a pseudospherical surface Σ.

Starting from it we can obtain several constitutive laws for specifical practical problems.

In particular, let us introduce into (2.19) the stress representation

$$\sigma = \sqrt{1+X^2}\tan\left[\frac{\sqrt{1+X^2}}{a}(c-c_0)\right], \tag{2.21}$$

In this case we get

$$\varepsilon = \frac{a^2}{2(1+X^2)}\left[\frac{c-c_0}{a} + \frac{1}{\sqrt{1+X^2}}\right]\sin\left(\frac{2\sqrt{1+X^2}}{a}(c-c_0)\right). \tag{2.22}$$

Thus, the relations (2.21) and (2.22) give a parametric representation of the constitutive laws $\sigma = \sigma(\varepsilon, X)$, for which the equations (2.1) are associated to a pseudospherical surface Σ.

These equations lead to

$$\sigma_{XX} = \varepsilon_{tt}. \tag{2.23}$$

Using (2.16), we have

$$\sigma_{XX} = \left[\frac{a^2}{(1+\sigma^2+X^2)^2}\sigma_t\right]_t. \tag{2.24}$$

The equation (2.24) has a solitonic behavior and admits soliton solutions (Munteanu and Donescu [14], [15]). These solutions, known as *solitons*, have the form of localized functions that conserve their properties even after interaction between them, and then act somewhat like particles. The equation (2.24) like other remarkable equations (Korteweg and de Vries, Burgers, sine-Gordon, Schrödinger, etc.) has interesting properties: an infinite number of local conserved quantities, an infinite number of exact solutions expressed in terms of the Jacobi elliptic functions (*conoidal solutions*) or the hyperbolic functions (*solitonic solutions* or *solitons*), as well as the simple formulae for nonlinear superposition of explicit solutions. Such equations were considered *integrable* or more accurately, *exactly solvable*. Given a nonlinear equation, it is natural to ask whether it is integrable, or it admits the exact solutions or solitons, whether its solutions are stable or not. This question is still open, and efforts are made to collect the main results concerning the analysis of nonlinear equations such as (2.24).

3 The Inverse Problem

The mathematical modelling is focused on the extracting or abstracting the essential feature from the complexities of the physical phenomena. The only way to justify the model is to show that what is predicted by it corresponds to some aspects of a real problem. The formulation of the constitutive property for a material is not formalism. A constitutive law must describe the global mechanical properties of the specimen, being an inverse problem, which cannot be treated empirically.

The inverse problem is an important subject in mechanics. Inverse problems are dealing with the determination of the mechanical system with unknown material properties from the knowledge of the measured responses to given loadings or excitations on its boundary. The inverse problem may be modelled into a parameter identification problem in which an optimal set of parameters should be found by minimizing an appropriate norm of differences between the computational responses and measured ones (Tanaka and Nakamura [16], Chiroiu and Chiroiu [17]).

We assume that the unknown three parameters $p = \{a, c, c_0\}$ from (2.22) are discretized into discrete values with the step width Δa, Δc, Δc_0. The set $p = \{a_{,i}, c_{,j}, c_{0,k}\}$ of parameters for an arbitrary problem is expressed as the combination number $M_{ijk} = (i-1)JK + (j-1)K + k$, where I, J, K are total number of discretized values for each parameter p. This number is counted from the first set of parameter $p = \{a_{,1}, c_{,1}, c_{0,1}\}$. We define the objective function as a square sum of differences between the experimental and the computed stress-strain results for carbon nanotubes

$$W = \sum_{m=1}^{M} (\sigma_i^m - \bar{\sigma}_i^m)^2, \tag{3.1}$$

where $\bar{\sigma}_i^m$ denotes the measured stress at point m on the experimental strain-stress diagram σ-ε, and σ_i^m denotes the computed strain-stress σ-ε at the same point m. M

is the number of points from the experimental uniaxial diagram σ-ε. We define fitness $\tilde{F}$ as a reciprocal number of the function W

$$\tilde{F} = \frac{W_0}{W}, \tag{3.2}$$

where

$$W_0 = \sum_{m=1}^{M} (\bar{\sigma}_i^m)^2. \tag{3.3}$$

As the convergence criterion of iterative computations by using a genetic algorithm, we use a non-dimensional expression

$$Z = \frac{1}{2} \log_{10} \frac{W}{W_0}. \tag{3.4}$$

For all considered examples, the number of populations is 25, ratio of reproduction 1, number of multi-point crossovers 1, probability of mutation 0.25 and the maximum number of generations 300.

We study the stretching and compression of the single-walled carbon nanotubes by varying the lattice parameter, along the tube axis. We impose a periodic boundary condition along the axial tube direction. The others cell parameters are 50 times the circular tube diameter D. The thickness of the tube wall is $h = 0.34$ nm, and the number of carbon atoms per a slab of width L is $N = 2\pi\rho LR$, where R is the radius of the tube and ρ – the density.

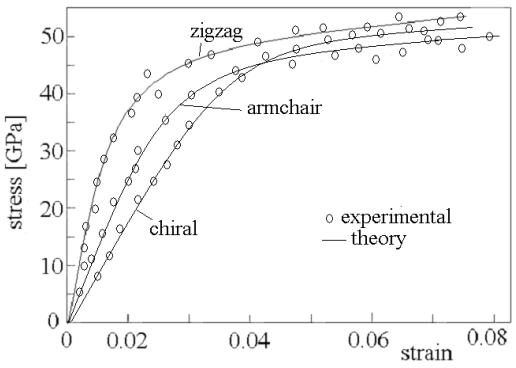

Fig. 3.1. The stress–strain law for different single–walled carbon nanotubes.

The constitutive law for the single-walled carbon nanotubes (armchair (10, 10) with radius $R = 3.223$ Å, chiral (12, 6) with $R = 4.553$ Å, and zigzag (17, 0) with $R = 6.264$ Å) obtained by the present inverse analysis, are illustrated in Fig. 3.1. The continuous line means the theoretical results and circles, the experimental results reported by Gao, Cagin and Goddard [18]. The results demonstrate that the pseudospherical reduction method coupled with a genetic algorithm can be successfully and efficiently applied to the identification of the constitutive laws for carbon nanotubes.

The results reveal the importance of the parameters a, c and c_0 in describing the stress-strain curve for carbon nanotubes. We can say that the parameter a is proportional to the radius R of the carbon nanotube for specified c and c_0. Also, the parameter c is proportional to the number n^2 which defines the nanotube, for specified a and c_0. Also, we can say that the parameter c_0 depends on $\sqrt{h}$ for specified a and c. An interesting case of a constitutive law, associated to a Ţiţeica surface (K/d^4 is constant), is considered for a chiral nanotube (18, 9) with $R = 6.222$ Å. We obtain the diagrams illustrated in Fig. 3.2, that show a significant ductility and fracture toughness

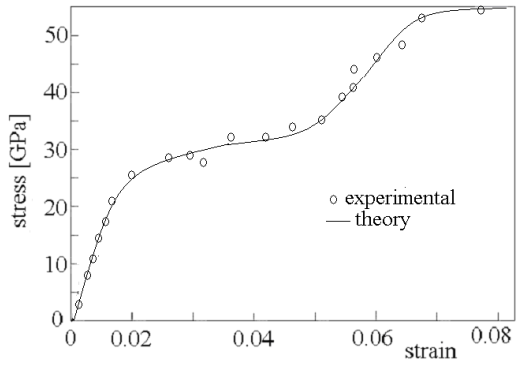

Fig. 3.2. The stress–strain law for a chiral nanotube (18, 9).

4 Conclusions

This paper is studying the mechanical properties of the single-walled carbon nanotubes with different radius and chirality forms (armchair (n, n), chiral $(2n, n)$, and zigzag $(n, 0)$), and perfect circular cross section, subjected to tensile loading. The goal of the paper is to determine a parametrical representation for a class of constitutive laws for which the motion equations attached to a material system is associated to a pseudospherical surface. The uniaxial deformation problem for the carbon nanotubes is discussed via the pseudospherical reduction technique. The parametric representation of the constitutive laws, for which the motion equations are associated to a pseudospherical surface, are given by (2.21) and (2.22), in terms of three parameters a, c and c_0.

A genetic algorithm is performed to study several inverse problems associated to experimental results. The relation of a to the Gaussian curvature is $K = -\frac{1}{a^2}$. So, we can conclude that if the motion equations can be associated to a pseudospherical surface Σ, of Gaussian curvature K, the strength of the carbon nanotube can be described as a function of K. The results yields to the conclusion that the parameter a is proportional to the radius R of the carbon nanotube for specified c and c_0. Another result is that the parameter c may be proportional to the number n^2 which defines the nanotube, for specified a and c_0, and the parameter c_0 depends on $\sqrt{h}$ for specified a and c.

A subclass of the constitutive laws is associated to a Ţiţeica surface, for which the ratio K/d^4 (d is the distance from the origin to the tangent plane at an arbitrary point) is constant. For carbon nanotubes, the parameter a is related to d, and it is important in describing the ductility and fracture toughness properties.

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