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MODELLING OF CARBON NANOTUBES BEHAVIOUR WITH THE USE OF A THIN SHELL THEORY

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In the paper, various problems connected with the possibility of modelling of single walled carbon nanotubes as thin cylindrical shells are discussed. The interatomic potentials playing the fundamental role in the description are presented. Special attention is focused on various types of nonlinearities (geometrical and material). The open problems arising in the modeling are also emphasised.

Key words: carbon nanotubes, shells, interatomic potential

1. Introduction

The investigations on carbon nanotubes behaviour have been mainly focused on the experimental description and molecular dynamics simulations such as classical molecular dynamics, tight-binding molecular dynamics and the ab initio method. However, the researchers have been seeking more efficient computational methods with which it is possible to analyse the large scale of CNTs in a more general manner. Yakobson *et al.* (1996) found that the continuum shell model could predict all changes of buckling patterns in atomistic molecular-dynamics simulations. The analogousness of the cylindrical shell model and CNTs leads to extensive application of the shell model for CNT structural analysis. Ru (2000a,b, 2001) used the CM approach and simulated the effect of van der Waals forces by applying a uniformly distributed pressure field on the wall, the pressure field was adjusted so as to give the same resultant force on each wall of the tube. It has verified that the mechanical responses of CNTs can be efficiently and reasonably predicted by the shell model provided that the parameters, such as Young's modulus and effective wall thickness, are judiciously adopted. Wang *et al.* (2006) studied buckling of double-walled carbon nanotubes under axial loads, by modeling

CNTs using solid shell elements. Han *et al.* (2003, 2006) investigated torsional buckling of a DWNT and MWNT embedded in an elastic medium. Han *et al.* (2005) also studied bending instability of double-walled carbon nanotubes. Yao and Han (2006, 2007) analysed the thermal effect on axially compressed and torsional buckling of a multi-walled carbon nanotube. Some conclusions were drawn that at low and room temperature the critical load for infinitesimal buckling of a multi-walled carbon nanotube increases as the value of temperature change increases, while at high temperatures the critical load for infinitesimal buckling of a multi-walled carbon nanotube decreases as the value of temperature change increases. Nonlinear postbuckling behaviour of carbon nanotubes under large strain is significant to whoch great attention is paid by some researchers (Wang *et al.*, 2005; Leung *et al.*, 2006). The torsional postbuckling behaviour of single-walled or multi-walled carbon nanotubes was discussed in details by Yiao and Han (2008).

The problems encountered in the numerical modelling of pristine and defective carbon nanotubes were demonstrated in details by Muc (2009, 2010). In the mentioned references, the linear and nonlinear (iterative) approaches were illustrated.

A successful work has been also conducted with continuum modelling such as dynamic studies. A comprehensive review of the literature dealing with the analysis of wave propagation in CNTs with the use of shell theories was presented by Liew and Wang (2007), although the authors focused the attention mainly on the application of thick shell theories. They pointed out that there was growing interest in the terahertz physics of nanoscale materials and devices, which opened a new topic on phonon dispersion of CNTs, especially in the terahertz frequency range. Hu *et al.* (2008) proposed to use nonlocal shell theories in the analysis of elastic wave propagation in single- or double-walled carbon nanotubes. However, it is worth to emphasise that the vibrational characteristics of CNTs are studied with the use of both beam theories and different variants of shell theories – see e.g. Natsuki *et al.* (2008) and Ghorbanpourarani *et al.* (2010). Recently, thermal vibrations have attracted considerable attention – see e.g. Tylikowski (2008), where the dynamic stability analysis was conducted with the use of stochastic methods. The cited above work demonstrates also another tendency in the dynamic analysis of multi-walled CNTs connected with the application of a multiple-elastic shell model which assumes that each of the concentric tubes of multiwall carbon nanotubes is an individual elastic shell and coupled with adjacent tubes through van der Waals interaction. The broader discussion of that class of problems was presented e.g. by Xu and Wang (2007).

The aim of the present paper is to discuss various problems encountered in the modelling of single-walled carbon nanotubes as continuous cylindrical thin shells.

2. Inter-atomic relations

At the beginning of our considerations, let us introduce basic relations describing carbon-carbon (C-C) interactions. They characterise physical bahaviour of carbon nanotubes, being in fact atomistic structures, and are fundamental in the further transformation from molecular dynamics relations to continuum (shell) mechanics.

The structure of nanotubes is obtained by conformational mapping of a graphene sheet onto a cylindrical surface. The nanotube radius is estimated by using the relation

$$R = r_0 \frac{\sqrt{3(m^2+n^2+mn)}}{2\pi} \tag{2.1}$$

where $r_0 = 0.141\,\mathrm{nm}$ is the carbon-carbon distance. The integers n and m denote the number of unit vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ along two directions in the honeycomb crystal lattice of graphene. If $m = 0$, they are called "zigzag" nanotubes; if $n = m$, they are called "armchair" nanotubes. For any other values of n and m, the nanotubes are called "chiral" because the chains of atoms spiral around the tube axis instead of closing around the circumference.

To capture the essential feature of chemical bonding in graphite, Brenner (1990) established an interatomic potential (called as the REBO potential) for carbon in the following form

$$V(r_{ij}) = V_R(r_{ij}) - B_{ij}V_A(r_{ij}) \tag{2.2}$$

where r_{ij} is the distance between the atoms i and j, V_R and V_A are the repulsive and attractive pair terms (i.e., depending only on r_{ij}), and are given by

$$V_R(r) = \frac{D_{(e)}}{S-1}\exp[-\sqrt{2S}\beta(r-R)] \qquad V_A(r) = \frac{D_{(e)}S}{S-1}\exp\Big[-\sqrt{\frac{2}{S}}\beta(r-R)\Big] \tag{2.3}$$

In the above expression, the cut-off function is assumed to be equal to 1 to avoid a dramatic increase in the interatomic force.

The parameter B_{ij} in Eq. (2.2) represents the multibody coupling between the bond from the atoms i and j and the local environment of the atom i, and is given by

$$B_{ij} = \Big[1 + \sum_{k(\neq i,j)} G(\theta_{ijk})\Big]^{-\delta} \tag{2.4}$$

where θ_{ijk} is the angle between bonds $i-j$ and $i-k$, and the function G is given by

$$G(\theta) = a_0\Big[1 + \frac{c_0^2}{d_0^2} + \frac{c_0^2}{d_0^2 + (1+\cos\theta)^2}\Big] \tag{2.5}$$

and the term B_{ij} is expressed in the symmetric form

$$\overline{B}_{ij} = \frac{1}{2}(B_{ij} + B_{ji}) \tag{2.6}$$

The set of material parameters is adopted here as follows

$$\begin{aligned} &D_e = 0.9612\,\mathrm{nN\,nm} && S = 1.22 && \beta = 21\,\mathrm{nm}^{-1} \\ &R = 0.139\,\mathrm{nm} && \delta = 0.5 && a_0 = 0.00020813 \\ &c_0 = 330 && d_0 = 3.5 \end{aligned} \tag{2.7}$$

In contrast to the REBO potential function, in which the bond stretch and bond angle are coupled in the potential, Belytschko *et al.* (2002) proposed the modified Morse potential function, which can be expressed as the sum of energies that are associated with the variance of the bond length $V_{stretch}$, and the bond angle V_{angle}, i.e.

$$\begin{aligned} &V = V_{stretch} + V_{angle} \\ &V_{stretch} = D_e\{[1 - \exp(-\beta(r - r_0))]^2 - 1\} \\ &V_{angle} = \frac{1}{2}k_\theta(\theta - \theta_0)^2[1 + k_{sextic}(\theta - \theta_0)^4] \end{aligned} \tag{2.8}$$

The material constants are following

$$\begin{aligned} &r_0 = 1.421 \cdot 10^{-10}\,\mathrm{m} && D_e = 9 \cdot 10^{-19}\,\mathrm{Nm} \\ &\beta = 1.8 \cdot 10^{10}\,\mathrm{m}^{-1} && \theta = 120^\circ \\ &k_\theta = 0.9 \cdot 10^{-18}\,\mathrm{Nm/rad}^2 && k_{sextic} = 0.754\,\mathrm{rad}^{-4} \end{aligned} \tag{2.9}$$

By differentiating Eq. (2.2) or Eq. $(2.8)_1$, the stretching force of atomic bonds is obtained. The force variations with the bond length are almost the same while

the bond angle is kept constant as $2\pi/3$. However, for the REBO potential, the force varies with the bond angle variations, whereas for the modified Morse potential it is always constant. Thus, the inflection point (force peak) is not constant for the REBO potential. As it is reported, both bond lengths and bond angles vary as CNTs are stretched. Therefore, in our numerical model, it is necessary to consider two possible formulations of interatomic potentials to analyse and compare the influence of those effects on the nonlinear behaviour and fracture strain.

From the interatomic potentials that are shown in Eqs. (2.2) and $(2.8)_1$, the stretching force that results from the bond elongation and the twisting moment that results from the bond angle variation can be calculated as follows

$$F(r_i) = \frac{\partial V}{\partial r_i} \qquad M(\theta) = \frac{\partial V}{\partial \theta} \tag{2.10}$$

Figure 1a compares the interatomic stretching force for the REBO and modified Morse potentials in the tensile regime, whereas Fig. 1b shows the bond angle moment for the REBO and modified Morse potentials. Let us note that they present nonlinear behaviour.

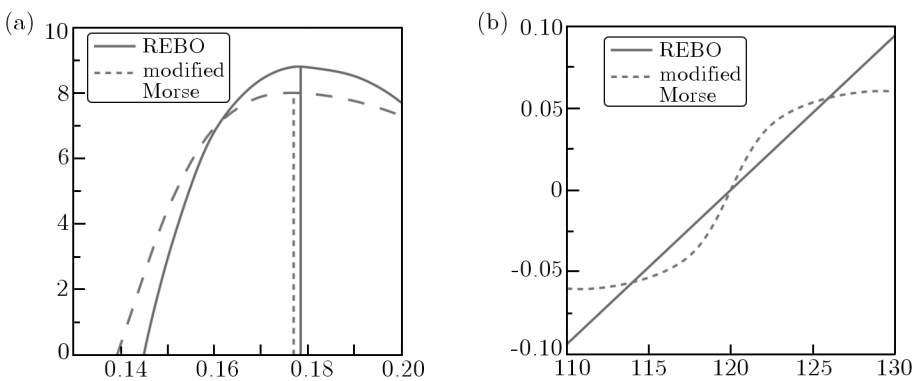

Fig. 1. Tensile (a) force and (b) moment distributions

3. Continuum shell model

To describe mechanical behaviour of carbon nanotubes in the form of classical shell relations, it is necessary to introduce the equivalent Young modulus E and the equivalent shell thickness h – Fig. 2.

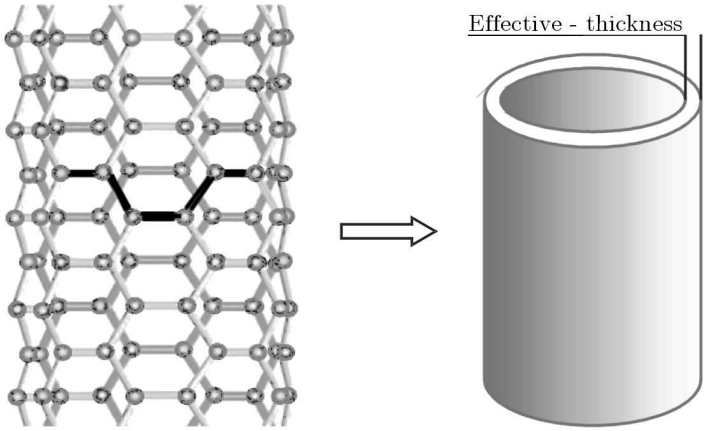

Fig. 2. Continuum model of carbon nanotube structure

In general, three different approaches are possible:

- to assume the above-mentioned values; for instance Yakobson *et al.* (1996) suggested that the effective Young modulus is 5.5 TPa and the wall thickness of the carbon nanotube is 0.066 nm based on their SWCNT buckling results obtained by MD simulation and the continuum mechanics shell model
- to fit the results to atomistic simulation results of tension rigidity $EA = Eh/(1-\nu^2)$ and bending rigidity $EI = Eh^3/[12(1-\nu^2)]$, where ν is the Poisson ratio; this gives (Huang *et al.*, 2006))

$$h = \sqrt{12\frac{EA}{EI}} = 3\sqrt{2\Big(\frac{\partial V}{\partial \cos\theta_{ijk}}\Big)_0\Big(\frac{\partial^2 V}{\partial r_{ij}^2}\Big)_0^{-1}} \tag{3.1}$$

- to determine analytically tensile, shear, bending and torsional rigidities directly from the interatomic potential, and therefore avoid any fitting not-well-defined elastic modulus and thickness (Wu *et al.*,2008). This atomistic-based shell theory gives the relation among the increments of second Piola-Kirchhoff stress $\mathbf{T}$, moment $\mathbf{M}$, Green strain $\mathbf{E}$, and curvature $\mathbf{K}$ as

$$\mathbf{T} = \mathbf{L} : \mathbf{E} + \mathbf{H} : \mathbf{K} \qquad \mathbf{M} = \mathbf{H} : \mathbf{E} + \mathbf{S} : \mathbf{K} \tag{3.2}$$

where $\mathbf{L}$, $\mathbf{H}$ and $\mathbf{S}$ are the fourth-order rigidity tensors obtained analytically from the interatomic potential.

Using the above-mentioned approaches, it is possible to evaluate buckling loads of cylindrical shells, analyse their post-buckling behaviour, etc., just employing the methods of analysis well-known for shell problems. In this way, it is possible to describe the behaviour of equivalent carbon single-walled or multi-walled carbon nanotubes. However, there is always an open question dealing with the accuracy and correctness of such approaches. Some of those problems will be discussed in the next section.

4. Open problems

Peng *et al.* (2008) determined the order of error for approximating single-walled carbon nanotubes by a thin shell. The ratio of atomic spacing r_0 to the single-walled carbon nanotubes radius R (i.e. r_0/R), is used to identify the order of error. They considered the structural response of single-walled carbon nanotubes subject to tension (or compression), torsion, bending and internal (or external) pressure. They proved that only for the order of error equal to 40%-(5.5) armchair single walled carbon nanotubes can be modelled as thin shells with constant thickness and isotropic mechanical properties.

The extensions of the above results were presented by Wu *et al.* (2008). The authors defined degrees of: anisotropy, nonlinearity and coupling, i.e., down to the radius of single-walled carbon nanotubes at which the tension/bending coupling becomes negligible in constitutive relation (3.2).

Numerical modelling of single-walled carbon nanotubes constitutes a separate class of problems. Some of them were discussed by Kalmakarov *et al.* (2006). The cited work presents also the comparison of Young's modulus and the equivalent thickness predicted with the use of various theories.

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Zastosowanie teorii powłok w zagadnieniach modelowania deformacji nanorurek węglowych

Streszczenie

W artykule przedstawiono problematykę modelowania deformacji jednościennych nanorurek węglowych przy pomocy teorii cienkościennych powłok cylindrycznych. W opisie zastosowano teorię potencjałów oddziaływań międzyatomowych. Szczególną uwagę zwrócono na kwestie opisu nieliniowości geometrycznych i fizycznych. Podkreślono także istnienie wielu nierozwiązanych do chwili obecnej zagadnień związanych z modelowaniem deformacji nanorurek.

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