CAPTUREMENT OF THE NANOSCOPIC MORPHOLOGICAL PARAMETERS IN CHIRAL SWCNT'S VIA A WELL-POSED CONTINUUM MODEL

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1. General

The natural angle of twist within a chiral free-standing single-walled carbon nanotube (SWCNT) as well as the natural extension along the axis of a chiral and achiral CNTs can remarkably alter both the mechanical and electronic properties of these nano-structures. The current work provides an exact analysis within the mathematical framework of continuum mechanics for large deformations. The initial elastic fields (the natural angle of twist and the natural extension) within a free-standing CNT which is merely induced by bending of graphene have been commonly neglected in the continuum-based treatments of these nano-structures. For an accurate prediction of the mechanical response of CNT subjected to subsequent loadings, it is essential to account for these residual elastic fields. Just to give a perception, the SWCNT (9,3) with diameter of 0.85 nm and chirality angle of β=13.9° has a natural angle of twist of about 1.81×10^{-3} rad/nm and natural extension of about 2.4×10^{-4} nm per unit length. Accounting for these parameters and utilizing an enhanced constitutive equation, the ideal tensile and hoop strengths as well as the stiffness in the axial-, hoop-, and radial-directions for the chiral SWCNTs will be determined.

2. Roll up of graphene into SWCNT and the induced initial elastic fields

In the framework of the present work, graphene which is a one-atom-thick layer of carbon densely packed in a honey-comb-shaped lattice is treated as a lamina. It can undergo large elastic deformations. Also, in this work a SWCNT obtained by rolling up of graphene is referred to as the elastica, [1,2]. Some geometrical details of graphene (lamina) and the corresponding SWCNT (elastica) are given in Figs. 1(a) and (b), respectively.

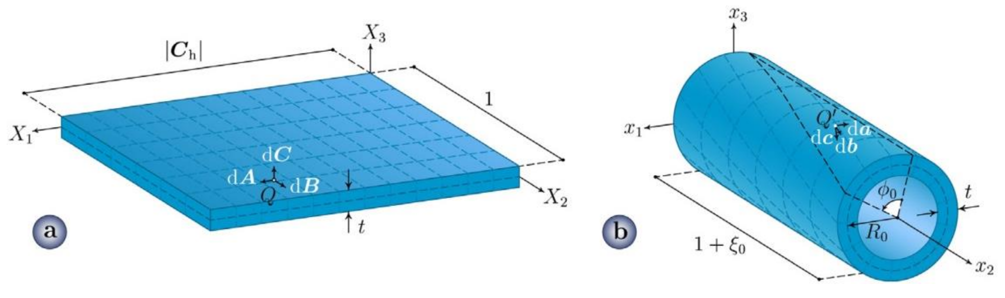

Fig. 1. Geometry of (a) unit strip of graphene (lamina), and (b) the obtained SWCNT (elastica).

Consider a strip of graphene (lamina) with dimensions $1\times|\boldsymbol{C}_h|\times t$, where $\boldsymbol{C}_h$ denotes the chirality vector and t the thickness. The origin of the Lagrangian coordinates (X_1, X_2, X_3) is set on the mid-plane of the lamina as shown in Fig. 1(a). By bending the lamina of unit length about the X_2-axis, the SWCNT (elastica) with length not equal to 1 but equal to $1+\xi_0$ as shown in Fig. 1(b) is obtained. ξ_0 is the natural extension of the free-standing elastica. In general, this operation is accompanied with a relative rotation of the two ends of the tube which is referred to as the natural angle of twist. Let ϕ_0 and R_0 denote the natural angle of twist and the mean radius of the CNT, respectively. It is noteworthy to mention that, due to the presence of the residual elastic fields $R_0\neq|\boldsymbol{C}_h|/2\pi$. Graphene is a one atom thick layer and it is reasonable to assume that it is not deformable in its thickness direction. Thus, t=0.0883 nm ([1]) for the lamina and elastica is the same. For a SWCNT with the structural index (n,m) the magnitude of the chirality vector is given by $|\boldsymbol{C}_h|=\sqrt{3}a_0\sqrt{n^2+mn+m^2}$, where a_0=1.412Å is the length of the carbon-carbon bonds in graphene. Select a set of Eulerian coordinates (x_1, x_2, x_3) associated with the CNT shown in Fig. 1(b) in such a way that its origin coincides with the center of the tube's cross-section and, moreover, the tube's axis lies along the positive direction of the x_2-axis.

The equation of equilibrium with respect to the reference coordinates (X_1, X_2, X_3) are given by

(1) $$\frac{\partial}{\partial X_j}\left(\sigma_{jk}\frac{\partial x_i}{\partial X_k}\right)=0,$$

where $\boldsymbol{\sigma}$ is the second Piola-Kirchhoff stress tensor. Consideration of the equilibrium of a free-standing tube results in a system of integral equations for the morphological parameters (R_0, ξ_0, ϕ_0).

3. Numerical results and conclusion

If the tube is subjected to external loadings then the integral equations must be modified accordingly for the unknown morphological parameters (R, ξ, ϕ). The extension-induced twist, ϕ (rad/nm) as a function of axial engineering strain for CNT (3n,n) with β=13.9° is shown in Fig. 2. The pressure-induced twist versus hoop strain for the same CNT is given in Fig. 3.

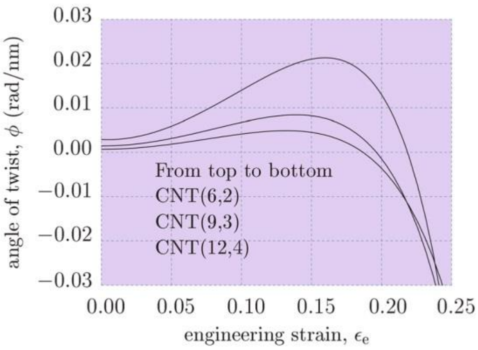

Fig. 2. Extension-induced twist versus axial engineering strain.

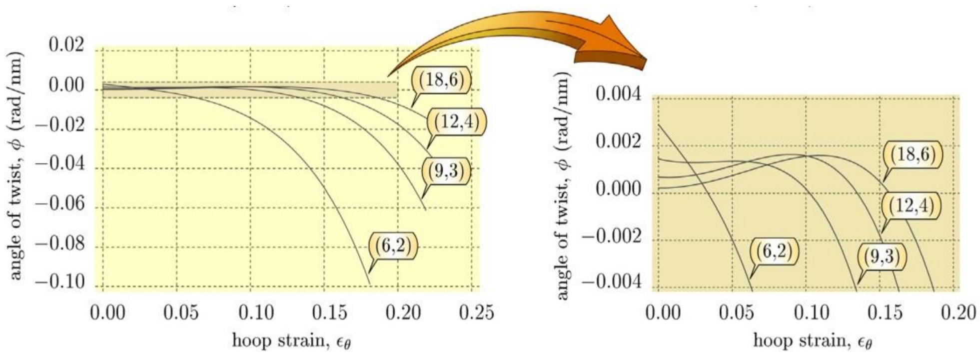

Fig. 3. Pressure-induced twist versus hoop strain.

4. References

[1] M.R. Delfani, H.M. Shodja and F. Ojaghnezhad (2013). Mechanics and morphology of single-walled carbon nanotubes: from graphene to the elastica, *Phil. Mag.*, **93**, 2057–2088.

[2] M.R. Delfani and H.M. Shodja (2015). An exact analysis for the hoop elasticity and pressure-induced twist of CNT-nanovessels and CNT-nanopipes, *Mech. Mat.*, **82**, 47–62.