

## **An atomistic-continuum elastic rod model of carbon nanotubes**

Karthick CHANDRASEKER, Subrata MUKHERJEE\*

\*Cornell University  
220 Kimball Hall, Ithaca, NY 14853.  
[sm85@cornell.edu](mailto:sm85@cornell.edu)

### **Abstract**

The present work focuses on an atomistic-continuum model of single-walled carbon nanotubes (SWNTs) based on an elastic rod theory (Healey [1]) which can exhibit geometric as well as material nonlinearity. In particular, the SWNT is modeled as a one-dimensional elastic continuum which has some finite thickness bounded by the lateral surface. Exploitation of certain symmetries in the underlying atomic structure leads to suitable representations of the continuum elastic energy (Healey [1]). The bridging between the atomic scale and the effective continuum is carried out by parameterization of the continuum elastic energy and determination of the parameters using atomistic simulations.

### **1. Introduction**

Continuum elastic behavior of SWNTs has often been characterized using properties such as Young's and shear moduli. These linearized measures adequately describe material behavior under small strains. However, in SWNTs undergoing large strains, there are effects such as the coupling between extension and twist (Chandraseker and Mukherjee [2]) which are not captured by linearized, isotropic moduli. While this is an evidence of anisotropy in large strains, it is of interest to also characterize other deformation couplings in SWNTs. The following are the key contributions of the present work:

- The proposed rod model for SWNTs in this work takes into account: (a) bending (b) twist (c) shear (d) extension (e) coupled extension and twist, and (f) coupled bending and shears. Published work on elastic moduli has taken into account (a)-(d) individually for small strains, and past work (including Chandraseker and Mukherjee [2]) has considered (e). But this is the first effort at a unified large strain approach that takes into account all of these modes for SWNTs.
- While two-dimensional membrane models of SWNTs (e.g., Chandraseker and Mukherjee [2]; Arroyo and Belytschko [3]) have been useful to predict localized effects such as buckled mode shapes of the effective continuum, they may not be computationally efficient to model global behavior of long tubes (microns in length) of interest in nano-oscillators (see, for e.g. Sazonova *et al.* [4]; Ustunel *et al.* [5]). A one-dimensional model is better suited to such an application. However, one-dimensional models published so far are limited to linear stress-strain relationships with isotropic material assumptions which do not take into account the aforementioned couplings.
- Finally, since this is a parameterized continuum model of an atomic system, it is possible to apply this model, by suitable parameter estimation, to other atomic systems such as silicon or boron nitride nanotubes.

## 2. Special Cosserat rod: Basic kinematics and constitutive model

It is assumed that the reference configuration of the rod is straight with a prismatic cross-section and that plane sections remain plane after deformation. (Rods that are initially bent - a common situation in practice - can be modeled by extending the theory presented below). Referring to Figure 1, one has:

$$\mathbf{x} = \mathbf{f}(\mathbf{X}) = \mathbf{r}(s, t) + X_\alpha \mathbf{d}_\alpha(s, t)$$

with  $\mathbf{X} = X_\alpha \mathbf{e}_\alpha + s \mathbf{e}_3$     Here  $s = X_3$

(1)

In the above,  $\mathbf{X}$  and  $\mathbf{x}$  are undeformed and deformed coordinates, respectively,  $s = X_3$  is the arc length in the reference configuration,  $t$  is time,  $\mathbf{r}$  is the position vector of a point on the rod centerline in the deformed configuration,  $\mathbf{e}_\alpha$  are Cartesian unit vectors and  $\mathbf{d}_\alpha$  are director vectors that span the cross-section (assumed to be planar). Summation is implied on all repeated indices and the range of Greek indices such as  $\alpha$  is 1, 2.

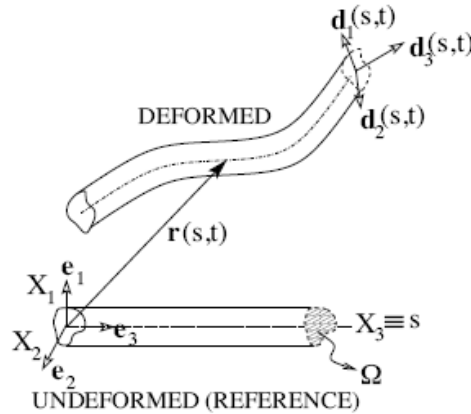


Figure 1: Cosserat rod notation

A special Cosserat theory is employed in which:

$$\mathbf{d}_i \cdot \mathbf{d}_j = \delta_{ij}, \quad \mathbf{d}_3 = \mathbf{d}_1 \times \mathbf{d}_2, \quad \mathbf{d}_i(s, t) = \mathbf{R}(s, t) \mathbf{e}_i, \quad i = 1, 2, 3$$

(2)

where:  $\delta_{ij}$  are the components of the Kronecker delta and the matrix  $\mathbf{R}$  represents the rotation of the cross-section of the rod. Based on the above kinematic description, one can define strains as follows:

$$\mathbf{r}_{,s}(s, t) = v_i \mathbf{d}_i(s, t)$$

(3)

where:  $v_1, v_2$  are shear strains, and  $v_3$  is the axial stretch (axial strain =  $v_3 - 1$ ).

Further,

$$\begin{aligned} \mathbf{d}_{i,s}(s, t) &= \mathbf{R}_{,s}(s, t) \mathbf{e}_i = \mathbf{R}_{,s} \mathbf{R}^T \mathbf{d}_i \\ &\equiv \mathbf{K} \mathbf{d}_i(s, t) = \boldsymbol{\kappa} \times \mathbf{d}_i(s, t) \end{aligned}$$

(4)

where:  $\kappa_1, \kappa_2$  are measures of the bending curvatures, and  $\kappa_3$  is a measure of the twist.

It can be shown that the most general quadratic representation of the strain energy density for hemitropic, flip symmetric rods (see Healey [1] for definitions and details) is of the form:

$$W = \frac{1}{2} \left[ A \kappa_\alpha \kappa_\alpha + B \kappa_3^2 + C v_\alpha v_\alpha + D (v_3 - 1)^2 + 2E (v_3 - 1) \kappa_3 + 2F v_\alpha \kappa_\alpha \right] \quad (5)$$

where  $\int_0^L W ds$  gives the total elastic energy stored in a rod of undeformed length 'L' for a given deformation specified by  $v_i, k_i$  ( $i = 1, 2, 3$ ). The parameters 'A' through 'F' are coupling coefficients and represent the different coupling effects in bending, shear, extension and twist of the rod. For example, the coefficient 'E' represents the extension-twist coupling which has been studied previously (see, for e.g., Chandraseker and Mukherjee [2]).

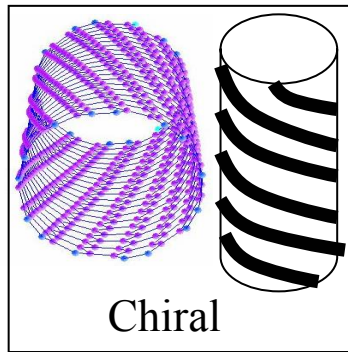


Figure 2: Helical idealization of a chiral SWNT

## 2.1 Helical symmetry

SWNTs can be shown to possess a helical atomic arrangement as illustrated in Figure 2 (zigzag and armchair SWNTs can be modeled as special cases of this helical atomic arrangement).

It is observed that rods possessing a single-helical structure exhibit a special flip symmetry (180-degree rotation invariance) about a unique axis passing through the intersection of the helix with a plane perpendicular to the rod axis (as illustrated in Figure 3) at any point along the axis. This symmetry axis "rotates" as we move from cross-section to cross-section along the length of the rod (see Figure 3).

Further, in the case of chiral nanotubes, the atomic arrangement can be viewed as comprising of multiple helices (see Figure 2). In this case, there exist two or more equally spaced symmetry axes (see Figure 3). Consequently, it can be shown (Healey [1]) that for rods exhibiting n-fold multiple helical symmetry with  $n \geq 3$  (which is true for any realistic chiral nanotube), the most general *quadratic* strain energy density is identical to the case of hemitropy + flip symmetry, i.e. the strain energy density function up to quadratic order is the same as Eq. (5). Since armchair and zigzag nanotubes can be treated as special cases of a chiral SWNT, the above description also applies to such nanotubes.

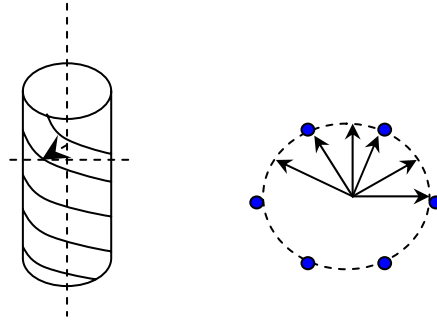


Figure 3: Single and multiple (for  $n = 6$ ) helical symmetries

Hence, a continuum SWNT rod model up to quadratic order is immediately realized once the parameters ‘A’ through ‘F’ in Eq. (5) can be evaluated for SWNTs.

### 3. Summary

In order to extract the coefficients ‘A’ through ‘F’, unit cell simulations of extension, twist, bending and shear deformations are performed using a self-consistent-charge density-functional-tight-binding approach (see, for e.g., Frauenheim *et al.* [6]). The strain measures for the rod model are extracted using the atom locations to define cross-sections for the rod model. Using the extracted strains and the relaxed cell energies, the coefficients in Eq. (5) are evaluated through a least-squares fitting procedure. The key results from simulations on a (9,6) SWNT are:

- The quadratic extension-twist coupling coefficient ‘E’ can be shown to be zero.
- The shear modulus (a measure of stiffness to rotations of cross-sections about axes in-plane) can be shown to be approximately equal to the twist modulus, each of which is around 35-40% of the Young’s modulus.
- The bending rigidity can be shown to be of the order of 1.65-2.3% of a Bernoulli-Euler beam prediction indicating that direct application of a continuum beam model to SWNTs can significantly overestimate the bending stiffness.

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