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# ON THE APPLICATION OF CHEBYSHEV POLYNOMIALS TO NANOROPES TWIST

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A coupled atomistic-continuum theory for describing the twist of nanoropes is proposed in this article. The model couples a region described with full atomistic detail to a surrounding region modeled with the continuum concepts. The shifted Chebyshev polynomials of the second kind and a generalization of Vekua and Nikagadze methods are performed on the base of a nonclassical parametrization of the transition region.

*Key words:* Nanoropes, Chebyshev polynomials, Nonclassical parametrization.

## 1. INTRODUCTION

The concept of the space elevator was introduced by russian scientist Konstantin Tsiolkovsky in 1895, based on the Eiffel Tower in Paris. This space elevator must be able to launch objects into orbit without a rocket. The Tsiolkovsky's concept is a compression structure, rather than a tension structure. After the development of carbon nanotubes in the 1990s, it was realized that the small dimensions, strength and remarkable mechanical properties of carbon nanotubes make them a very unique material which might make the concept of an orbital skyhook feasible [1]-[6].

Generally, the nanoropes are made from fullerene single-wall carbon nanotubes. These materials are produced of more than 70 percent by condensation of a laser-vaporized carbon-nickel-cobalt mixture at 1200°C. X-ray diffraction and electron microscopy showed that these carbon nanotubes are nearly uniform in diameter and that they self-organize into ropes, which consist of 100 to 500 carbon nanotubes in different arrangements. Fig. 1.1 shows such a carbon nanotube rope made from 6 subropes, each subrope being composed from 7 groups of single wall carbon nanotubes. Each group contains 25 carbon nanotubes with two different radii (zigzag and armchair 6.26A, $h$ = 0.617A and 16.33A, $h$ = 0.998A), and the core group consists of 49 chiral carbon nanotube with the same radius (3.22A and $h$ = 0.6A), into a polymeric matrix.

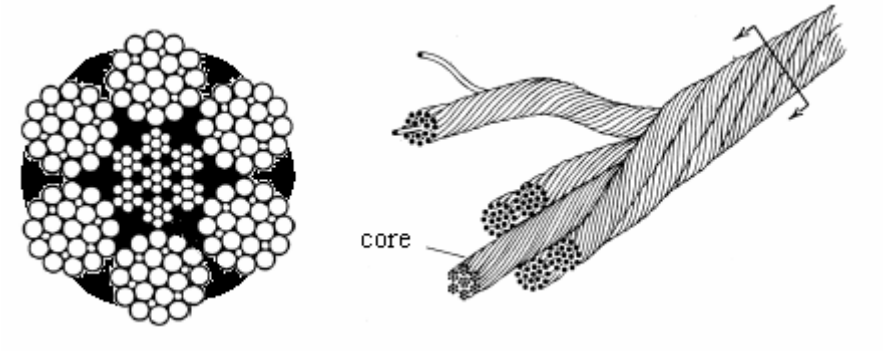


Fig. 1.1. The structure of nanorope.

In this paper, a coupled atomistic-continuum theory is performed for describing the twist of nanoropes made from single-walled carbon nanotubes [7]-[10]. The model couples a region described with full atomistic detail to a surrounding region modeled with the continuum concepts. The shifted Chebyshev polynomials of the second kind and a generalization of Vekua and Nikagadze methods are performed on the base of a nonclassical parametrization of the transition region.

## 2. CHEBYSHEV POLYNOMIALS

The polynomial Chebyshev of second kind on the interval $[-1,1]$ are given by [11]-[13]

$$U_n(x)=[1/(n+1)]T'_{n+1}(x)\,,\ -1\le x\le 1\,,\ n\in \mathrm{N}_0\,. \tag{2.1}$$

In (2.1), $T_n(x)=\cos(n\arccos x)$ are the Chebyshev polynomials of the first kind, and $\mathrm{N}_0$ is a set of natural numbers. The shifted Chebyshev polynomials are defined as

$$U^*_n(t)=U_n(2t-1)=\{1/[2\sqrt{t(1-t)}]\}\sin[(n+1)\arccos(2t-1)]\,,\ 0\le t\le 1\,.$$

The functions

$$F^*(r,t)=1/[1+r)^2-4rt]\,,\ h^*(x)=2\sqrt{2(1-t)}\,,\ |r|\le 1\,,\ 0\le t\le 1\,, \tag{2.2}$$

are the generating and weighting functions for these polynomials .

To obtain the basic recurrence relations, the first can be derived for $U_n(x)$ and then for $U^*_n(t)$ by substituting $2t-1\,,\ 0\le t\le 1$ for $x$. As a result, it is obtained

$$\begin{gathered}4tU^*_n(t)=U^*_{n-1}(t)+2U^*_n(t)+U^*_{n+1}(t)\,,\\ 2tU^{*\prime}_n(t)=2nU^*_n(t)+2U^*_{n-1}{}'(t)+U^{*\prime}_n(t)\,,\ n\ge 1\,,\\ U^{*\prime}_n(t)=4nU^*_{n-1}(t)+U^*_{n-2}{}'(t)\,,\ n\ge 2\,.\end{gathered} \tag{2.3}$$

On the base of (2.3) additional recurrence relations are obtained

$$2^{2s}t^sU^*_k(t)=\sum_{p=0}^{2s}C^p_{2s}U^*_{k-s+p}(t)\,,\ k-s\ge 0\,,\ k\in \mathrm{N}_0\ , \tag{2.4}$$

$$2^{2(k+1)}t^{k+1}U^*_k(t)=\sum_{p=0}^{2k+2}C^p_{2k+2}U^*_{p-1}(t)\,,\ k\in \mathrm{N}_0\ , \tag{2.5}$$

$$2^{2(k+s)}t^{k+s}U^*_k(t)=-\sum_{q=2}^{s}C^{q-2}_{2k+2s}U^*_{s-q}(t)+\sum_{p=s}^{2k+2s}C^p_{2k+2s}U^*_{p-s}(t)\,,\ k\in \mathrm{N}_0\ ,\ s\ge 2\,, \tag{2.6}$$

$$2^{2s}t^sU^*_m(t)U^*_n(t)=\sum_{p=0}^{m}\ \sum_{q=0}^{2s}C^q_{2s}U^*_{n-m-s+2p+q}(t)\,,\ \ n-m-s\ge 0\,, \tag{2.7}$$

$$U^{*\prime}_n(t)=4\sum_{k=0}^{[(n-1/2]}(n-2k)U^*_{n-(2k+1)}(t)=4\sum_{k=0}^{[(n-1/2]}(2k+1+a)U^*_{2k+a}(t)\,,\ n\ge 1\,, \tag{2.8}$$

$$U_n^{*\prime\prime}(t) = 2^4 \sum_{k=0}^{[(n-1/2]} (k+1)(n-k)(n-2k-1)U_{n-(2k+2)}^*(t)$$
$$= 2^2 \sum_{k=0}^{[(n-2/2]} (2k+2-a)[(n+1)^2-(2k+2-a)^2]U_{2k+1-a}^*(t), \quad n \geq 2, \tag{2.9}$$

In these expressions $a = n-1-2\left[(n-1)/2\right]$ with $[x]$ the integer part of $x$. The expressions (2.3)-(2.9) with the exception of (2.7) contain the orthogonal Chebyshev polynomials $\{\widehat{U}_k^*\}_{k=0}^{\infty}$ of the second kind, defined as $\widehat{U}_k^* = \| U_n^* \|^{-1} U_k^*$, with $U_n^*$ the shifted polynomial Chebyshev of second kind on the interval [0,1] and $\| U_k^* \| = \sqrt{\pi}/2$, the norm of $U_k^*$. Relation (2.7) can be written for orthogonal polynomials as

$$2^{2s} t^s U_m^*(t) U_n^*(t) = \widehat{U}_0^* \sum_{p=0}^{m} \sum_{q=0}^{2s} C_{2s}^q \widehat{U}_{n-m-s+2p+q}^*(t), \quad n-m-s \geq 0. \tag{2.10}$$

## 3. MACROSCOPIC AND MICROSCOPIC MODELING

At the macrosopic, the carbon nanorope is modeled as a rod of length l, with circular cross section of radius less than its length $a << l$. A new parametrization is applied to the region occupied by the body $x \in [-a,a]$, $s \in [0,l]$, for a given time interval $t \in [0,T]$. Instead of $x \in [-a,a]$ we can use $x \in [0,1]$. For any integrable function $A(x,s)$, $x \in [0,1]$, $s \in [0,l]$, $t \in [0,T]$, we consider an expansion of the form

$$A(x,s,t) = \sum_{k=0}^{\infty} A^{(k)}(s,t) \widehat{U}_k^*(x), \quad x \in [0,1], \; s \in [0,l], \; t \in [0,T], \tag{3.1}$$

where $A^{(k)}(s,t)$ is the $k$th coefficient in the expansion of $A(x,s,t)$ in the orthonormal Chebyshev polynomials $\{\widehat{U}_k^*(x)\}_{k=0}^{\infty}$ of the second kind. Let us to consider the integral

$$I^{(k)}(A) = \int_0^1 A(x,s,t) \widehat{U}_k^*(x) h(x) \mathrm{d}x, \quad k \in \mathrm{N}_0 \; s \in [0,l], \tag{3.2}$$

where $h(s)$ is a properly chosen weighting function. This integral verifies the property of linearity

$$I^{(k)}[\alpha(s)A + \beta(s)B] = \alpha(s) I^k(A) + \beta(s) I^k(B), \tag{3.3}$$

for any functions $A$ and $B$ of the form (3.1). Also, it is easily to show that $I^{(k)}(A)$ defined by (3.3) is equal to the $k$th coefficient in the expansion of $A$ in these polynomials with respect to $x$

$$I^{(k)}(A) = \int_0^1 A(x,s,t) \widehat{U}_k^*(x) h(x) \mathrm{d}x = A^{(k)}(s,t), \text{ with } k \in \mathrm{N}_0. \tag{3.4}$$

External moments fix the ends of the tube. At the macroscopic scale, we know the motion of the rod between $t = 0$ and $r_{ij}$ if and only if we know the mapping $S(0,t), \; \forall t \in [0,t_1]$, which takes a material point in $\Omega_0$ at $t = 0$ to a spatial position in $\Omega(t)$ at $t = t_1$. The mapping is single valued and possess continuous partial derivatives with respect to their arguments. The position of a material point in $\Omega_0$ may be denoted by a rectangular fixed coordinate system $X \equiv (X,Y,Z)$ and the spatial position of the same point in $\Omega(t)$, by the moving coordinate system $x \equiv (x,y,z)$. The motion of the rod carries various material points through various spatial positions. The curvature $C$, in the longitudinal direction, the nondimensional curvature $c$, the deformation parameter $\zeta$, are defined as

$$C=\frac{2ch}{\sqrt{3}R^2(1-\nu^2)},\quad c=\frac{\sqrt{3\zeta}}{2}\ ,\ \zeta=\frac{R-R_c}{R},\tag{3.5}$$

where $R$ and $R_c$, are the radius before and after deformation. The strain energy per unit length $\Pi$ is given by

$$\Pi=\Pi_0+\frac{1}{2}\pi R^3hC^2E\sum_{k=1}a_k\zeta^k,\ \Pi_0=\frac{3\pi Eh\hat{h}^2\zeta^2}{8R}+\frac{5\pi Eh\hat{h}^2\zeta^4}{16R},\ \hat{h}=\frac{h}{\sqrt{1-\nu^2}}.\tag{3.6}$$

The energy (3.6) can be expressed under the form (3.1)

$$\Pi(x,s,t)=\frac{1}{2}\sum_{k=0}^{\infty}L^{(k)}(s,t)\widehat{U}_k^*(x),\tag{3.7}$$

where $x_c\in[0,1]$, $s_c\in[0,l]$ represents the region occupied by the body, where the continuum theory is valid, for $t\in[0,T]$. In (3.7), $L^{(k)}(s,t)$ is the $k$th coefficient in the expansion of $\Pi(x,s,t)$ in the orthonormal Chebyshev polynomials $\{\widehat{U}_k^*(x)\}_{k=0}^{\infty}$ of the second kind. These coefficients can be calculated with (3.4). The total energy of the tube $\Pi_t$ and the bending moment $M$ can be written as $\Pi_t=\Pi l$, $M=\frac{\mathrm{d}\Pi_t}{\mathrm{d}\vartheta}$, where $\vartheta$ is the bending angle. The critical compressive stress $\sigma_{cr}=\frac{N}{h}$, where $N$ is the axial load, and the critical bending moment $M_{cr}$ in local buckling can be also calculated. This theory is valid up to the point of local buckling at a specific value for the bending angle $\vartheta$.The elastic energy is the bending and twisting of each nanotube summed over all nanotubes. For unit nanorope length, bending and torsional energies of each nanotube depends on its bending and torsional stiffness $EI$ and $GJ$. The total energy of the twisted rope is expressed as a function of the bulk twist angle $\phi$.

Secondly, the atomistic modeling of the bar is analyzed. The total atomic energy $E^a$ can be expressed as a sum of individual atom energies. The energy of an atom is

$$E_i^a=F_i(\bar{\rho}_i)+\frac{1}{2}\sum_{j\neq i}\alpha_iV_{ij}(r_{ij}),\tag{3.8}$$

where $F_i$ is an electron-density dependent embedding energy, $V_{ij}$ is a pair potential between $i$-th and $j$-th and $r_{ij}$ is the interatomic distance, and $\alpha_i$ unknown constants. The electron density at atom $i$, $\bar{\rho}_i$ is the superposition of density contributions from each of the neighbours $\bar{\rho}_i=\sum_{j\neq i}\rho_j(r_{ij})$.

The van der Waals force refers to the attractive or repulsive forces between molecules or between parts of the same molecule, other than those due to covalent bonds or to the electrostatic interaction of ions with one another or with neutral molecules. In this article this force is introduced to model the interaction between the opposite walls of the nanotube when they approach each other. This force depends on the distance between the atoms. For large distances, the van der Waals force is attractive, but when the separation between the atoms is below the critical equilibrium distance, it becomes strongly repulsive. The van der Waals force between atom $i$ and $j$ can be expressed by the Lennard-Jones 6-12 potential as

$$V_{ij}(r_{ij})=A\left(\frac{1}{2}\frac{d_0^6}{r_{ij}^{12}}-\frac{1}{r_{ij}^6}\right).\tag{3.9}$$

where $A=24.3\times10^{-79}\,\mathrm{Jm}^6$ and $d_0=0.383\mathrm{nm}$ are parameterized to describe interlayer forces in graphite [14], [15]. For the energy field $E^a(x,s)$ we consider an expansion of the form (3.1)

$$E^a(x,s)=\sum_{k=0}^{\infty}E^{a(k)}(s)\widehat{U}_k^*(x)\,, \tag{3.10}$$

where $x_a\in[0,1]$, $s_a\in[0,l]$ represents the region where the atomistic theory is valid. In (3.3), $E^{a(k)}(s)$ is the *k*th coefficient in the expansion of $E^a$ in the orthonormal Chebyshev polynomials $\{\widehat{U}_k^*(x)\}_{k=0}^{\infty}$ of the second kind. These coefficients can be calculated with (3.4).

For nanoropes, the inclusion of non-bonded interactions is important, because this explains the inter tube rotational mode as a result of long range van der Waals forces.

Thirdly, the transition region between continuum and atomistic regions are modeled. On one side of the transition boundary is the atomistic region in which every atom is explicitly represented and treated by using interatomic potentials. The transition or boundary region between the atomistic and continuum regions is a very important aspect of the modelling.

At the interface between the atoms and the nodes of the continuum region, we construct a one-to-one correspondence with the aid of the Chebyshev polynomials of the second kind. The parametrization of the transition region $x_{tr}\in[0,1]$, $s_{tr}\in[0,l]$ is constructed such that the following assertion is valid.

*Assertion. The energy field $E^{tr}(x,s)$ of the transition region verifies the conditions*

$$E^{tr}(x,s)\to E^c(x,s)\text{ for }x_{tr}\to x_c\,,\ s_{tr}\to s_c \tag{3.11}$$

*and*

$$E^{tr}(x,s)\to E^a(x,s)\text{ for }x_{tr}\to x_a\,,\ s_{tr}\to s_a\,, \tag{3.12}$$

*where*

$$E^{tr}(x,s)=\sum_{k=0}^{\infty}E^{tr(k)}(s)\widehat{U}_k^*(x)\,, \tag{3.13}$$

*with* $x_{tr}\in[0,1]$, $s_{tr}\in[0,l]$.

In (3.13) $E^{tr(k)}(s)$ is the *k*th coefficient in the expansion of $E^{tr}(x,s)$ in the orthonormal Chebyshev polynomials $\{\widehat{U}_k^*(x)\}_{k=0}^{\infty}$ of the second kind. These coefficients can be calculated as

$$E^{(k)tr}(s)\to\int_0^1 E^a(x,s)\widehat{U}_k^*(x)h_a(x)\mathrm{d}x\,,\ k\in\mathrm{N}_0\text{, for }x_{tr}\to x_a\,,\ s_{tr}\to s_a\,, \tag{3.14}$$

and

$$E^{(k)tr}(s)\to\int_0^1 E^c(x,s)\widehat{U}_k^*(x)h_c(x)\mathrm{d}x\,,\ k\in\mathrm{N}_0\text{, for }x_{tr}\to x_c\,,\ s_{tr}\to s_c\,, \tag{3.15}$$

with unknown functions $h_a(x)$ and $h_c(x)$ that are determined from an inverse problem such that (3.11) and (3.12) hold.

The total potential energy of the coupled atomistic-continuum model is obtained by summing the energies associated with the atomistic, continuum and transition regions as

$$\begin{gathered}E(x,s)=E^c(x_c,s_c)+E^a(x_a,s_a)+E^{tr}(x_{tr},s_{tr})\,,\ (x_c,s_c)\in I_c\,,\ (x_a,s_a)\in I_a\,,\ (x_{tr},s_{tr})\in I_{tr}\\ I_c\cup I_a\cup I_{tr}=[0,1]\times[0,l]\,,\ I_i\cap I_j=O\,,\ i,j=a,c,tr\,.\end{gathered} \tag{3.16}$$

## 4. RESULTS

The elastic moduli of nanotubes used in the calculations are $E$ = 1.347 TPa and $G$ = 0.547 TPa, and the bending and torsion stiffness are calculated based on a main nanotube thickness 0.34 nm [16], [17]. The assertion (3.11)-(3.13) is verified by calculating the equilibrium bulk twist $\phi_{eq}$ at the interface between the atomistic and continuum regions. As we see in fig. 4.1, the nonclassical parametrization assures a good continuity of solutions.

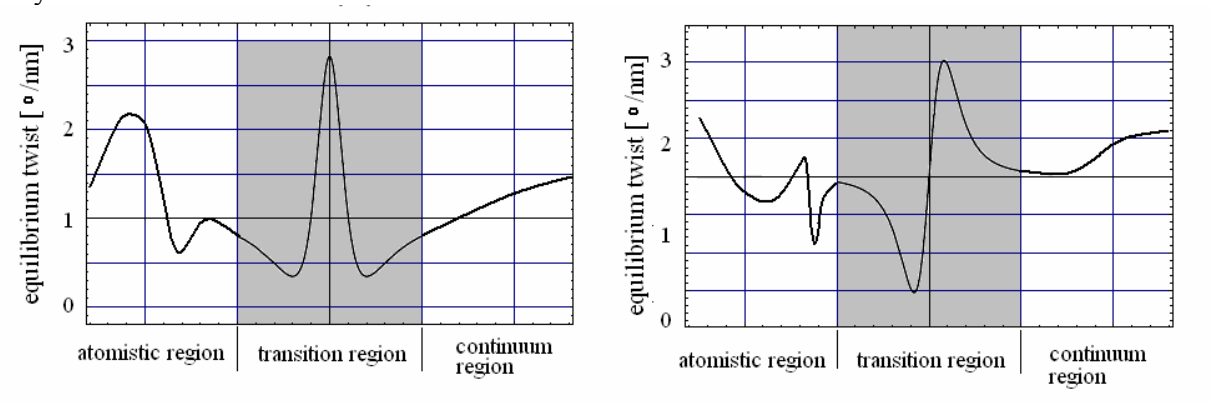


Fig. 4.1 The variation of the equilibrium twist at the transition region for a nanorope of radius 48nm (left ) and 50nm (right).

Fig. 4.2 shows the rope radius dependence of the equilibrium bulk twist $\phi_{eq}$ with the nanorope radius $R$. The behavior of nanorope at twisting can be divided into three distinct regimes, separated by dotted lines [17]. In regime I, defined by $R < R_1 = 40\text{nm}$, it is no twist. Regime II is defined by $40\text{nm} = R_1 \le R \le R_2 = 52\text{nm}$, and is characterized by a stable twist. The regime III for $R > 52\text{nm}$, shows unabated twist. The last region has to be investigated in details because here, the stored elastic energy is too small to offset the enhanced cohesive energy of the nanorope. Ideally, the crystal should continually twist, but in practice, as explained Liang and Upmanyu [17], the prediction is the nanorope dissembles into smaller radii nanoropes.

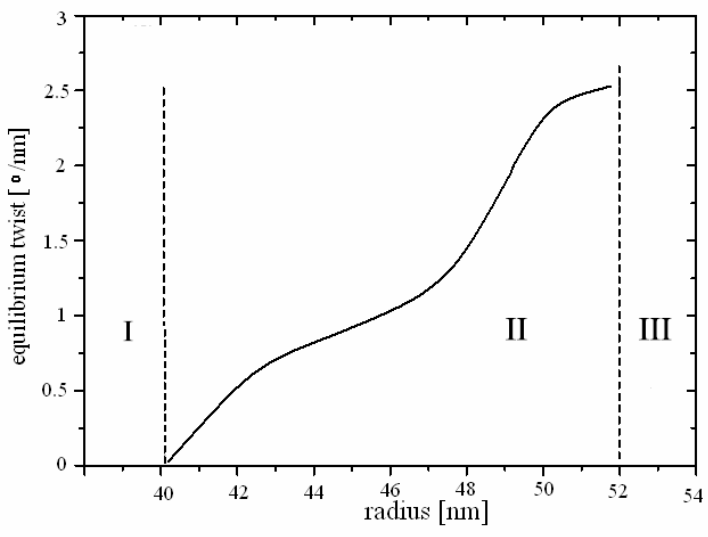


Fig. 4.2. The rope radius dependence of the equilibrium bulk twist with the nanorope radius.

## 4. CONCLUSIONS

In this paper, a coupled atomistic-continuum theory is performed for describing the twisting of nanoropes made from single-walled carbon nanotubes. The model couples a region described with full atomistic detail to a surrounding region modeled with the continuum concepts. The shifted Chebyshev polynomials of the second kind and a generalization of Vekua and Nikagadze methods are performed on the base of a nonclassical parametrization of the transition region. This study is motivated by the fact that while there are several advantages to forming bulk single crystals of carbon nanotubes, the assembly of them has been limited to rope radii less than 30 nm [17]. The results show a strong capacity of nanoropes for twisting, that makes nanoropes to be unprecedented candidates for the ultimate conductors for use in nanoscale devices.

We can say that the equilibrium and the stability of the nanorope twisting is a function of radius, and is determined by the competition between individual nanotube elastic deformations and the nanorope cohesive energy.

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