Study of axial strain-induced torsion of single-wall carbon nanotubes using the 2D continuum anharmonic anisotropic elastic model

Weihua Mu\textsuperscript{1,5}, Ming Li\textsuperscript{2}, Wei Wang\textsuperscript{3} and Zhong-can Ou-Yang\textsuperscript{1,4}

\textsuperscript{1} Key Laboratory of Frontiers in Theoretical Physics and Kavli Institute for Theoretical Physics China, Institute of Theoretical Physics, The Chinese Academy of Sciences, P O Box 2735, Beijing 100190, People’s Republic of China
\textsuperscript{2} Graduate University of Chinese Academy of Sciences, Beijing 100190, People’s Republic of China
\textsuperscript{3} College of Nanoscale Science and Engineering (CNSE), University at Albany, State University of New York, NY 12203, USA
\textsuperscript{4} Center for Advanced Study, Tsinghua University, Beijing 100084, People’s Republic of China
E-mail: muwh@itp.ac.cn

\textit{New Journal of Physics} \textbf{11} (2009) 113049 (10pp)
Received 4 August 2009
Published 25 November 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/11/113049

Abstract. Recent molecular dynamic simulations have found that chiral single-walled carbon nanotubes (SWCNTs) twist during stretching, resembling the motion of a screw. Obviously this phenomenon, as a type of curvature–chirality effect, cannot be explained by the usual isotropic elastic theory of SWCNTs. More interestingly, with larger axial strains (before buckling), the axial strain-induced torsion (a-SIT) shows asymmetric behaviors for axial tensile and compressing strains, which suggests the anharmonic elasticity of SWCNTs plays an important role in real a-SIT responses. In order to study the a-SIT of chiral SWCNTs with actual sizes, and to avoid possible deviation of computer simulation results due to the finite-size effect, we propose a two-dimensional (2D) analytical continuum model which can be used to describe SWCNTs of arbitrary chirality, curvature, and length, and which is concerned with their anisotropic and anharmonic elasticity. The elastic energy of the present model comes from the continuum limit of lattice energy based on second generation

\textsuperscript{5} Author to whom any correspondence should be addressed.
reactive empirical bond order potential (REBO-II), a well-established empirical potential for solid carbons. Our model has no adjustable parameters, except for those presented in REBO-II, and all the coefficients in the model can be calculated analytically. Using our method, we obtain the a-SIT responses of chiral SWCNTs with arbitrary radii, chiralities and lengths. Our results are in reasonable agreement with recent molecular dynamic simulations (Liang et al 2006 Phys. Rev. Lett. 96 165501). Our approach can also be used to calculate other curvature–chirality-dependent anharmonic mechanical responses of SWCNTs.

The extraordinary mechanical properties of carbon nanotubes (CNTs), such as high elastic modulus, exceptional directional stiffness, and low density, make them ideal for nanoelectromechanical systems (NEMS) devices [1]–[3]. Recent studies have demonstrated the possibility of using CNTs as actuators [4], nanotweezers [5], and nanorelays [6]–[9]. A detailed understanding of mechanical behavior, especially of the structurally specific mechanical properties of CNT-based NEMS devices, is therefore crucial for their potential use in NEMS.

Unlike with an isotropic elastic thin shell, due to the special geometry of single-walled carbon nanotubes (SWCNTs), e.g. chiralities, there is coupling between axial strain and torsion strain, which is similar to an ordinary helical spring [10]. More interestingly, recent molecular dynamic simulations found asymmetric behaviors of such coupling in chiral SWCNTs [11, 12] and double-walled carbon nanotubes (DWCNTs) [13], namely, asymmetry of axial strain-induced torsion (a-SIT) for tensile and compressing strains [11]. Later, Upmanyu et al.’s [14] finite element method simulation also obtained an asymmetrical a-SIT response. The main property of asymmetric a-SIT is that a-SIT responses for tension or compression are much different at large strain. Torsion angle per unit length increases when the strain increases in tension. However, with increasing strain under compression, the torsion angle firstly increases, then decreases to zero, and increases again after changing the direction of twist [11]–[13].

A-SIT implies the coupling between axial vibration modes and torsional ones for chiral SWCNTs, which may play an important role in the applications of CNT–NEMS oscillators [15, 16]. To understand an a-SIT responses, there are very few studies: Gartstein et al [10] used a two-dimensional (2D) continuum elastic model, and predicted a linear a-SIT effect for chiral SWCNTs with small strain, i.e. the SWCNT twists in opposite directions for tension and compression and the rotation angle varies linearly with strain. Gartstein et al [10] found that the a-SIT response is chirality dependent and that it reaches a maximum when the chiral angle is π/12. Liang and Upmanyu’s [11] molecular simulations extended the study of a-SIT to the large-strain region (before buckling), and obtained asymmetrical a-SIT. By comparing a-SIT response with changes of geometry of carbon–carbon bonds, they found asymmetrical a-SIT is relevant to the microscopic lattice structure of SWCNTs. Geng and Chang [12] studied both the torsion induced by axial strain and axial strain induced by torsion, and showed the nonlinear axial stress–strain relation occurring in the same time. Upmanyu et al.’s [14] finite element method simulation also obtained a-SIT.

All these efforts are valuable in understanding a-SIT. Nevertheless, Gartstein et al’s [10] theory was restricted to linear a-SIT responses, while the molecular dynamic or finite element method simulations for a series of SWCNTs with some special chiral index were time-consuming and substantial computer resources were needed, which limits their further application to the study of the properties of actual SWCNTs. In addition, there is a general caveat
to these simulation works: can the results of simulations for small systems be extrapolated to SWCNTs at equilibrium state with actual sizes?

To our knowledge, there is no easily handled theoretical framework capturing the basic physics of asymmetrical a-SIT which can obtain the responses for actual SWCNTs at equilibrium states with arbitrary radii and chiralities. To fulfill this task, we propose a quasi-analytical approach based on continuum elastic theory. In our model, the carbon–carbon interactions in SWCNTs are described by second generation reactive empirical bond order (REBO-II) potential \[17\], which is a classical many-body potential for solid carbon and hydrocarbons. The advantages of the REBO-II potential are that it has the analytical form of carbon–carbon pair potentials with the bond length and bond angle as variables of energy functions, and that the parameters of the REBO-II potential were fitted from a large data set of experiments and \textit{ab initio} calculations. The REBO-II potential can accurately reproduce the elastic properties of diamond and graphite, and in \[11\], the molecular dynamic simulation was also based on the REBO-II potential.

The carbon–carbon interaction energy near the equilibrium state without deformations can be obtained analytically by Taylor expansion with inclusion of the most important cubic term, i.e. anharmonic term of bond stretching,

\[ V = V_0 + \frac{1}{2} \sum_{\langle ij \rangle} \left( \frac{\partial V}{\partial r_{ij}^2} \right)_0 (r_{ij} - r_{ij}^0)^2 + \sum_{\langle ij \rangle} \sum_{k \neq i,j} \left( \frac{\partial^2 V}{\partial r_{ij} \partial \cos \theta_{ijk}} \right)_0 (r_{ij} - r_{ij}^0) (\cos \theta_{ijk} - (\cos \theta_{ijk})^0) \\
+ \frac{1}{2} \sum_{\langle ij \rangle} \sum_{k \neq i,j} \left( \frac{\partial^2 V}{\partial (\cos \theta_{ijk})^2} \right)_0 (\cos \theta_{ijk} - (\cos \theta_{ijk})^0)^2 \\
+ \sum_{\langle ij \rangle} \sum_{k,l \neq i,j} \left( \frac{\partial^2 V}{\partial \cos \theta_{ijk} \partial \cos \theta_{ijl}} \right)_0 (\cos \theta_{ijk} - (\cos \theta_{ijk})^0) \\
\times (\cos \theta_{ijl} - (\cos \theta_{ijl})^0) + \frac{1}{3!} \sum_{\langle ij \rangle} \left( \frac{\partial^3 V}{\partial r_{ij}^3} \right)_0 (r_{ij} - r_{ij}^0)^3. \tag{1} \]

Here \( \langle ij \rangle \) denotes the nearest-neighboring atom pairs, \( \theta_{ijk} \) denotes the angle between bonds \( i - j \) and \( i - k \). The equilibrium state is denoted by ‘0’. Similar series expansion for quadratic terms for the Brenner potential \[18\] has been reported by Huang \textit{et al} \[19\].

The non-crossing second and fourth terms in the right-hand side of equation (1) were also presented in Lenosky’s model \[20\]. From the analytical form of the REBO-II potential, the derivatives are,

\[ \left( \frac{\partial^2 V}{\partial r_{ij}^2} \right)_0 \approx 43.67 \text{ eV} \cdot \text{Å}^{-2}, \quad \left( \frac{\partial^2 V}{\partial r_{ij} \partial \cos \theta_{ijk}} \right)_0 \approx -5.924 \text{ eV} \cdot \text{Å}^{-1}, \]

\[ \left( \frac{\partial^2 V}{\partial (\cos \theta_{ijk})^2} \right)_0 \approx 3.187 \text{ eV}, \quad \left( \frac{\partial^2 V}{\partial \cos \theta_{ijk} \partial \cos \theta_{ijl}} \right)_0 \approx -0.367 \text{ eV}, \]

and

\[ \left( \frac{\partial^3 V}{\partial r_{ij}^3} \right)_0 \approx -333.4 \text{ eV} \cdot \text{Å}^{-3}. \]

\[ \text{New Journal of Physics 11 (2009) 113049 (http://www.njp.org/)} \]
In the 2D elastic theory of SWCNTs, the in-plane deformations of SWCNTs can be described by [22]

\[ \varepsilon = \begin{pmatrix} \varepsilon_1 & \varepsilon_6/2 \\ \varepsilon_6/2 & \varepsilon_2 \end{pmatrix}, \]

with \( \varepsilon_1 \equiv \varepsilon_{11}, \varepsilon_2 \equiv \varepsilon_{22}, \varepsilon_6 \equiv 2\varepsilon_{12} \), being the axial, circumferential, and shear strains, respectively. After deformation, the bond vectors from atom \( i \) to its three nearest neighboring atoms \( j \), deviate from the initial bond vector \( \vec{r}_{ij}^0 \),

\[ \vec{r}_{ij} \approx (1 + \varepsilon) \vec{r}_{ij}^0. \]

A SWCNT can be viewed as a cylinder with radius \( R \), and its surface can be perfectly embedded by six-member carbon rings [21]. There are three bond curves passing one carbon atom at the surface of a SWCNT; in the continuum limit, the bond vector can be written as [21]

\[ \vec{r}^0(M) = \hat{r}_{ij}^0 = \left[ 1 - a_0^2 \kappa^2(M)/6 \right] a_0 \hat{r}(M) + \left[ a_0 \kappa(M)/2 + a_0^2 \kappa_s(M)/6 \right] a_0 \tilde{N}(M) + \kappa(M) \tau(M) a_0^2 \tilde{t}(M), \]

where \( a_0 = 1.42 \text{ Å} \) is the carbon–carbon bond length without strain, \( M = 1, 2, 3 \) denotes three \( sp^2 \)-bonded curves from atom \( i \) to atom \( j \) on the surface of the SWCNT. Vectors \( \hat{r}, \tilde{N} \) and \( \tilde{t} \) are unit tangential, normal, and binormal vectors of the bond curves from atom \( i \) to \( j \); \( \kappa, \tau \) and \( s \) are the curvature, torsion, and arc parameter of bond curve, respectively, \( \kappa_s \equiv d\kappa/ds \) [21].

The vectors \( \hat{r}(M) = \cos \theta(M) \hat{e}_x + \sin \theta(M) \hat{e}_y, \tilde{N}(M) = \sin \theta(M) \hat{e}_x - \cos \theta(M) \hat{e}_y \), where \( \hat{e}_x \) and \( \hat{e}_y \) are the unit axial and circumferential vectors at the \( i \)-atom’s site on the SWCNT surface, while \( \theta(M) \) is the rotating angle from \( \hat{e}_x \) to tangent vector \( \hat{r} \), which is related to the chiral angle \( \theta_c \) [22].

After deformation, bond length \( r_{ij} = |\vec{r}_{ij}| \), and bond angle between bond vectors \( \hat{r}_{ij} \) and \( \hat{r}_{ik} \) is \( \cos \theta_{ijk} = \hat{u}_{ij} \cdot \hat{u}_{ik} \), with unit vector \( \hat{u}_{ij} \equiv \hat{r}_{ij}/r_{ij} \). Based on these relations, the 2D continuum limit of elastic energy per unit area of the SWCNT in equation (1), which avoids introducing ill-defined thickness of SWCNTs, can be written as,

\[ E_{\text{elasticity}} = \frac{1}{2} \sum_{ij} c_{ij} \varepsilon_i \varepsilon_j + \sum_{i \in j \in k} c_{ijk} \varepsilon_i \varepsilon_j \varepsilon_k, \]

where \( c_{ij} \) and \( c_{ijk} \) are in-plane elastic constants, \( i, j, k = 1, 2, 6 \), and they have analytical expressions (see the appendix). Among them, \( c_{16} \), the harmonic elastic constant for coupling between axial strain and torsional twist, is proportional to \( (a_0/R)^2 \sin(6\theta_c) \), which clearly shows that the a-SIT response is a curvature and chirality effect, which only occurs in chiral SWCNTs. Obviously linear a-SIT response is distinct at \( \theta_c = \pi/12 \) and significant for SWCNTs with small diameters, which is in accord with previous theoretical and simulation studies. For tubes with large diameters and small strains, anharmonic elastic energy can be ignored along with \( c_{16} \) and \( c_{26} \) terms, then the isotropic thin shell model for SWCNTs is recovered, and the calculated in-plane Young’s modulus and Poisson’s ratio are similar to the results in [22].

To study the asymmetrical a-SIT, we consider a chiral SWCNT with one fixed end, while the other end atoms are allowed to relax both radially and tangentially during deformation. The axial displacement is fixed for each simulation step, ensuring that only axial stress occurs, which is the basic assumption in simulations for a-SIT in SWCNTs [11, 12, 14].

The free energy per unit area of SWCNT under axial stress is

\[ F = E_{\text{elasticity}} - \sigma_1 \varepsilon_1. \]
Figure 1. Torsion angle–axial strain relations for a series of $(8, m), m = 0, 2, 4, 6, 8$ SWCNTs, which shows the chirality dependence of the a-SIT response. Only chiral SWCNTs $(8,2), (8,4)$ and $(8,6)$ have an a-SIT response, as shown.

Assumption of equilibrium state leads to the following nonlinear equations:

$$\frac{\partial \mathcal{F}}{\partial \varepsilon_i} = 0. \tag{5}$$

They give the relation between torsion angle per nm (in unit of degree) $\phi = -(180/\pi) \times \varepsilon_6/(R/1\text{nm})$ and axial strain $\varepsilon_1$, which is an asymmetrical response. There are two critical compressing strains $\varepsilon_1^*$ and $\varepsilon_1^{**}$, as shown in figure 1. For axial compression at $\varepsilon_1^*$, torsion angle reaches its extreme, then the SWCNT begins to untwist, and after totally untwisting at critical strain $\varepsilon_1^{**}$, the tube twists again in the opposite direction, i.e. in the same direction as that for the tension case.

Another interesting result is the nonlinear axial stress–strain relation; the axial secant Young’s modulus $Y_s \equiv d\sigma/d\varepsilon_1$ of the SWCNT is a strict monotonically decreasing function, $Y_s = Y_0 - t\varepsilon_1$, as shown in figure 2, thus SWCNTs show strain softening under tension, and strain hardening under compression. This phenomenon was also found in recent molecular dynamic simulations [12].

We find asymmetrical a-SIT and nonlinear axial stress–strain of SWCNTs are closely related to each other, the nature of which is anharmonicity of atom–atom interaction for SWCNTs, such as the REBO-II potential in [11] and in the present work. This anharmonicity leads to the anharmonic bond-stretching energy in equation (1) and the cubic terms in equation (3), (elastic energy).

To illustrate, we start from a simplified linear elastic energy per unit area of a SWCNT,

$$\tilde{\mathcal{F}} = \frac{1}{2} c_{11} \varepsilon_1^2 + c_{16} \varepsilon_1 \varepsilon_6 + \frac{1}{2} c_{66} \varepsilon_6^2 - \sigma_1 \varepsilon_1. \tag{6}$$

After substituting nonlinear stress–strain relation $\sigma_1 = Y_0 \varepsilon_1 - (t^2/2) \varepsilon_1^2$ to $\tilde{\mathcal{F}}$, using equilibrium condition $\partial \tilde{\mathcal{F}}/\partial \varepsilon_1 = 0$, the torsion angle, which is proportional to $\varepsilon_6$, is a quadratic function of

New Journal of Physics 11 (2009) 113049 (http://www.njp.org/)
Figure 2. The relation between in-plane axial secant Young’s modulus and axial strain, for a series of \((8, m)\), \(m = 0, 2, 4, 6, 8\) SWCNTs.

axial strain. The \(\phi(\varepsilon_1)\) curve is a parabola with its symmetric axial located at \(\varepsilon_1 < 0\). Thus, this analysis captures the main features of asymmetrical a-SIT.

Equation (3) without cubic terms gives the linear a-SIT response’s coefficient

\[
\frac{d\phi}{d\varepsilon_1} \bigg|_{\varepsilon_1=0} = \frac{c_{12}c_{26} - c_{22}c_{16}}{c_{22}c_{66}},
\]

with leading term \(\sim R^{-3}\) characterizing the linear a-SIT response, which is in good agreement with Gartstein et al’s [10] theoretical results. Therefore, the present analysis captures the main characteristics of the a-SIT response.

In our continuum elastic theory, we only get symmetrical a-SIT without anharmonic terms. However, Upmanyu et al [14] recorded asymmetrical a-SIT by finite element simulation based on harmonic elasticity, although it was a much smaller simulation (\(\sim 1/1000\) of those of molecular simulations). It may be because the elastic energy we used is the continuum limit of lattice energy, which may lose some subtle microscopic information. Our continuum elastic theory has some advantages, compared to previous simulations, because it is suitable to study SWCNTs with actual sizes, and all the elastic constants in the theory are obtained analytically. Obviously, our method can be extended to calculate other anharmonic properties of SWCNTs with arbitrary radii and chiralities.

In summary, we emphasize that anharmonicity of atomic interactions and curvature–chirality-induced anisotropic elasticity are both important in a-SIT response, and explain the asymmetrical a-SIT and nonlinear stress–strain relation. We find that the unusual asymmetrical a-SIT effects are the consequence of the curvature–chirality effect and of anharmonic elasticity. We give the analytical expressions of anharmonic elastic energy, as well as curvature–chirality-induced anisotropic elasticity based on the REBO-II. The calculated results are in reasonable agreement with recent molecular dynamic simulations. Our method can be used to calculate the anharmonic properties of SWCNTs with arbitrary radii and chiralities analytically.
Acknowledgments

We are grateful for helpful discussions with Dr H Liang, and Professors Y Wang and J Yan. We appreciate Dr Hangtao Lu’s careful reading of this paper.

Appendix

Elastic constants \( c_{11}, c_{12}, \ldots, c_{666} \) presented in equation (3) can be described by

\[
\mathbf{c} = \mathbf{Mb},
\]

where \( \mathbf{c} \) is a column vector with the components \( c_{11} \) to \( c_{46} \) being the 16 elastic constants of the SWCNT, i.e. \( c_{11} \) to \( c_{666} \), respectively, \( \mathbf{M} \) is a \( 16 \times 5 \) matrix, and \( \mathbf{b} \) is a column vector with the components,

\[
b_1 = \left( \frac{\partial^2 \mathbf{V}}{\partial \mathbf{r}^2_{ij}} \right)_0 \cdot \frac{a_0^2}{\Theta_0},
\]

\[
b_2 = \left( \frac{\partial^2 \mathbf{V}}{\partial (\cos \theta_{ijk})^2} \right)_0 \cdot \frac{1}{\Theta_0},
\]

\[
b_3 = \left( \frac{\partial^2 \mathbf{V}}{\partial \mathbf{r}_{ij} \partial \cos \theta_{ijk}} \right)_0 \cdot \frac{a_0}{\Theta_0},
\]

\[
b_4 = \left( \frac{\partial^2 \mathbf{V}}{\partial \cos \theta_{ijk} \partial \cos \theta_{ijl}} \right)_0 \cdot \frac{1}{\Theta_0},
\]

\[
b_5 = \left( \frac{\partial^3 \mathbf{V}}{\partial \mathbf{r}^3_{ij}} \right)_0 \cdot \frac{a_0^3}{\Theta_0}.
\]

Here, \( a_0 = 1.42 \, \text{Å} \) is the carbon–carbon bond length without strains, and \( \Theta_0 = 2.6 \, \text{Å}^2 \) is the area occupied by one carbon atom at the surface of a SWCNT.

All 34 nonzero elements of matrix \( \mathbf{M} \) are analytically written as

\[
M_{1,1} = \frac{9}{16} + \left( \frac{-45}{1024} \right) \alpha^2,
\]

\[
M_{2,1} = \frac{3}{16} + \left( \frac{-43}{1024} \right) \alpha^2 + \left( \frac{-11}{256} \right) \alpha^2 \cos(6\theta),
\]

\[
M_{3,1} = \frac{9}{16} + \left( \frac{-205}{1024} \right) \alpha^2 + \left( \frac{11}{128} \right) \alpha^2 \cos(6\theta),
\]

\[
M_{4,1} = \left( \frac{11}{512} \right) \alpha^2 \sin(6\theta),
\]

\[
M_{5,1} = \left( \frac{-33}{512} \right) \alpha^2 \sin(6\theta),
\]
\[ M_{6,1} = \frac{3}{16} + \left( \frac{-43}{1024} \right) \alpha^2 + \left( \frac{-11}{256} \right) \alpha^2 \cos(6\theta), \]
\[ M_{1,2} = \frac{27}{16} + \left( \frac{-27}{64} \right) \alpha^2 + \left( \frac{-189}{512} \right) \alpha^2 \cos(6\theta), \]
\[ M_{2,2} = \frac{-27}{16} + \left( \frac{27}{128} \right) \alpha^2 + \left( \frac{27}{64} \right) \alpha^2 \cos(6\theta), \]
\[ M_{3,2} = \frac{27}{16} + \left( \frac{-243}{256} \right) \alpha^2 \cos(6\theta), \]
\[ M_{4,2} = \left( \frac{-405}{1024} \right) \alpha^2 \sin(6\theta), \]
\[ M_{5,2} = \left( \frac{459}{1024} \right) \alpha^2 \sin(6\theta), \]
\[ M_{6,2} = \frac{27}{16} + \left( \frac{-27}{256} \right) \alpha^2 + \left( \frac{27}{64} \right) \alpha^2 \cos(6\theta), \]
\[ M_{1,3} = \frac{-9}{8} + \left( \frac{-285}{1024} \right) \alpha^2 + \left( \frac{-3}{64} \right) \alpha^2 \cos(6\theta), \]
\[ M_{2,3} = \frac{9}{8} + \left( \frac{-627}{1024} \right) \alpha^2 + \left( \frac{-3}{256} \right) \alpha^2 \cos(6\theta), \]
\[ M_{3,3} = \frac{-9}{8} + \left( \frac{-189}{1024} \right) \alpha^2 + \left( \frac{9}{128} \right) \alpha^2 \cos(6\theta), \]
\[ M_{4,3} = \left( \frac{-9}{512} \right) \alpha^2 \sin(6\theta), \]
\[ M_{5,3} = \left( \frac{-21}{512} \right) \alpha^2 \sin(6\theta), \]
\[ M_{6,3} = \frac{-9}{8} + \left( \frac{165}{1024} \right) \alpha^2 + \left( \frac{-3}{256} \right) \alpha^2 \cos(6\theta), \]
\[ M_{1,4} = \frac{-27}{32} + \left( \frac{27}{128} \right) \alpha^2 + \left( \frac{189}{1024} \right) \alpha^2 \cos(6\theta), \]
\[ M_{2,4} = \frac{27}{32} + \left( \frac{-27}{256} \right) \alpha^2 + \left( \frac{-27}{128} \right) \alpha^2 \cos(6\theta), \]
\[ M_{3,4} = \frac{-27}{32} + \left( \frac{243}{1024} \right) \alpha^2 \cos(6\theta), \]
\[ M_{4,4} = \left( \frac{-459}{2048} \right) \alpha^2 \sin(6\theta), \]
\[ M_{5,4} = \left( \frac{-459}{2048} \right) \alpha^2 \sin(6\theta), \]
\[ M_{6,4} = \frac{-27}{32} + \left(\frac{27}{512}\right) \alpha^2 + \left(\frac{-27}{128}\right) \alpha^2 \cos(6\theta), \]
\[ M_{7,5} = \frac{5}{64} + \left(\frac{1}{128}\right) \cos(6\theta), \]
\[ M_{8,5} = \frac{3}{64} + \left(\frac{-3}{128}\right) \cos(6\theta), \]
\[ M_{9,5} = \left(\frac{3}{128}\right) \sin(6\theta), \]
\[ M_{10,5} = \frac{3}{64} + \left(\frac{3}{128}\right) \cos(6\theta), \]
\[ M_{11,5} = \left(\frac{-3}{64}\right) \sin(6\theta), \]
\[ M_{12,5} = \frac{3}{64} + \left(\frac{-3}{128}\right) \cos(6\theta), \]
\[ M_{13,5} = \left(\frac{5}{64}\right) + \left(\frac{-1}{128}\right) \cos(6\theta), \]
\[ M_{14,5} = \left(\frac{3}{128}\right) \sin(6\theta), \]
\[ M_{15,5} = \left(\frac{3}{64}\right) + \left(\frac{3}{128}\right) \cos(6\theta), \]
\[ M_{16,5} = \left(\frac{-1}{128}\right) \sin(6\theta). \]

Here, \( \alpha \equiv a_0/R \).

References

[1] Baughman R H, Zakhidov A A and de Heer W A 2002 Science 297 787
[2] Craighead H G 2000 Science 290 1532
[3] Sapmaz S, Blanter Y M, Gurevich L and van der Zant H S J 2003 Phys. Rev. B 67 235414
[4] Baughman R H et al 1999 Science 284 1340
[5] Kim P and Lieber C M 1999 Science 286 2148
[6] Kinaret J M, Nord T and Viefers S 2003 Appl. Phys. Lett. 82 1287
[7] Lee S W et al 2004 Nano Lett. 4 2027
[8] Jang J E et al 2005 Appl. Phys. Lett. 87 163114
[9] Jang J E et al 2008 Appl. Phys. Lett. 93 113105
[10] Gartstein Y N, Zakhidov A A and Baughman R H 2003 Phys. Rev. B 68 115415
[11] Liang H and Upmanyu M 2006 Phys. Rev. Lett. 96 165501
[12] Geng J and Chang T 2006 Phys. Rev. B 74 245428
[13] Zhang H W, Wang L, Wang J B, Zhang Z Q and Zheng Y G 2008 Phys. Lett. A 372 3488
[14] Upmanyu M, Wang H L, Liang H and Mahajan R 2008 J. R. Soc. Interface 5 303
[15] Sazonova V et al 2004 Nature 431 284
[16] Zhao Y, Ma C-C, Chen G H and Jiang Q 2003 Phys. Rev. Lett. 91 175504
[17] Brenner D W, Shenderova O A, Harrison J A, Stuart S J, Ni B and Sinott S B 2002 J. Phys.: Condens. Matter 14 783
[18] Brenner D W 1990 Phys. Rev. B 42 9458
[19] Huang Y, Wu J and Hwang K C 2006 Phys. Rev. B 74 245413
[20] Lenosky T, Gonze X and Teter M 1992 Nature 355 333
[21] Zhong-can O-Y, Su Z-B and Wang C-L 1997 Phys. Rev. Lett. 78 4055
[22] Tu Z-C and Zhong-can O-Y 2002 Phys. Rev. B 65 233407