Mechanical and Electrical Properties of Single Walled Carbon Nanotubes: A Computational Study

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Abstract

Over the recent years, numerical modelling and computer based simulation of the properties of carbon nanotubes have become the focal points of research in computational nano-science. In this paper, we present the computational studies about the mechanical and transport properties of armchair (4, 4) and zigzag (4, 0) single walled carbon nanotubes (SWCNT). Unlike other materials, carbon nanotubes are so small that changes in structure can affect the Young’s modulus. Young's modulus for an armchair single-wall carbon nanotube and zigzag single-wall carbon nanotube are calculated using an atomistic approach and density functional theory (DFT). Atomic forces and total energies for strained carbon nanotube segments are computed using Atomistix's Virtual NanoLab (VNL) and ToolKit (ATK) software. For a maximum strain of one percent, elastic moduli are calculated using both force-strain and energy-strain data. The average values found for Young's modulus are in the range 1.8 to 4.17 TPa depending on the cross-sectional area taken for the carbon nanotube and the calculation method used. This is in good agreement with recent experimental findings. By using ab initio density functional theory (DFT) and non-equilibrium green function approach (NEGF), the structural and electronic properties such as electronic band structure, density of states (DOS) and transmission spectrum of the single walled carbon nanotube (SWCNT) are investigated. The results suggest a wide range for practical applications, such as NEMS, acoustic sensors and nano actuators.

Keywords: SWCNTs, DFT, NEGF, Young’s Modulus, Band gap, Zigzag, Armchair.

1. Introduction

Carbon Nanotube (CNT) structures are a recently discovered (1991) phase of carbon first synthesized in the laboratory of Sumio Iijima at Tsukuba [1]. They are known to exhibit a wide variety of electronic properties. They can be purely metallic or semiconducting. Semiconducting nanotubes are of particular interest for their potential industrial applications. CNTs are interesting because their strength and nanoscale size make them ideal for several applications in nanotechnology, electronics, optics, and
materials science. The carbon bonds in CNTs are similar to graphite, but their structure provides for bonds stronger than diamonds which give rise to the unique strength of CNTs [1]. The electronic properties of CNTs can also miniaturize the current micro scale in electronic devices. For example, CNT based transistors exist that operate at room temperature and can switch using a single electron [2]. Thus, high speed switches for future computers would require a fraction of the current that today's computers utilize and they would take up much less space than electronic components on today's CPU chips. Also, CNTs could result in high density storage for RAM applications since they can be miniaturized to scales far below current technologies.

Moreover, it is predicted that the switching time of these electronic components will be around a terahertz, which is 10,000 times faster than today's computers [3]. Future computers will be faster and orders of magnitude smaller with the new technology enabled by CNT-based transistors. CNTs have a low resistance which means they are great thermal conductors. Smaller diameter nanotubes can pack more tightly and carry larger amounts of current without overheating. Since they are great thermal conductors, they can also be used as heat sinks and transfer heat away from CPU chips [3]. Possible applications also include nanoscale electronic motors, mechanical memory elements, and Flexible nanotube films for use in computers and cell phones [2]. Tunable band gaps in nanomaterials could lead to full colour holographic projectors smaller than a postage stamp [2]. These projectors will offer a highly reliable touch screen, since CNTs are very flexible. Tunable band gaps can also give rise to lasers with a variable spectrum: by altering the band gap, the colour of the laser can change.

Moreover, it has been proposed that CNTs could possibly be used to transport genes in combination with radiofrequency fields to destroy cancer cells [4]. In addition, CNTs can be used in strain gauges in materials doped with CNTs that can sense tiny variations in internal strain in materials and relay that information optically, resulting in extremely fast failure detection in bridges, buildings, or other public infrastructure settings. Not only would the CNTs relay the stress information, but they would also improve the strength of the steel used in the construction. CNTs can even revolutionize everyday items such as clothes and sports gear where low weight and high strength is desired.

2. Molecular Structures of Nanotubes

2.1. Structure of the Bond

CNT is a cylindrical molecule composed of carbon atoms. A typical SWCNT structure is illustrated in Figure 1. A major feature of the structure is the hexagon pattern that repeats itself periodically in space. As a result of the periodicity, each atom is bonded to three neighboring atoms. Such structure is mainly due to the process of sp2 hybridization [5] during which one s-orbital and two p-orbitals combine to form three hybrid sp2 orbitals at 120° to each other within a plane (shown in Figure 2 for part of a graphene sheet). This covalent bond (referred to as the σ -bond) is a strong chemical bond and plays an important role in the impressive mechanical properties of CNT’s. In addition, the out-of-plane bond (the π-bond) that is relatively weak contributes to the interaction between the layers in MWCNTs, and between SWCNT’s in SWCNT bundles. Of course, the bonding is not purely sp2 in nanotubes, as curving the graphene sheet into a tube re-hybridizes the σ and π orbitals, yielding an admixture.

Figure 1: Molecular structure of a section of (10, 10) CNT. Each node shown is a carbon atom and lines are the chemical bonds.
Figure 2: Basic hexagonal bonding structure for one graphite layer (the ‘graphene sheet’). Carbon nuclei shown as filled circle, out-of-plane $\pi$-bonds, and $\sigma$-bonds connect the C nuclei in-plane.

2.2. Structures of Single-Walled Carbon Nanotube

As described above, the bonding in CNTs is similar, but not identical, to the graphene sheet. A widely used approach to identify the types of SWCNT is by reference to rolling up the graphene sheet. The key geometric parameter associated with this process is the roll-up vector $r$, which can be expressed as the linear combination of the lattice basis ($a$ and $b$).

Following the notation and Figure 3, we have:

$$r = na + mb.$$  \hspace{1cm} (1)

It is then possible to associate a particular integer pair ($n, m$) with each SWCNT. The relation between $n$ and $m$ also defines three categories of CNT:

- $m = 0$ & $\theta = 30^\circ$, ‘Zigzag’,
- $n = m$ & $\theta = 0^\circ$ ‘Armchair’,
- $n > m$ & $0 < \theta < 30^\circ$, ‘Chiral’

Figure 3: Definition of roll-up vector as linear combinations of base vectors $a$ and $b$. 
3. Computational Method - Ab Initio Molecular Dynamics Simulation Methods

In the section dealing with the classical molecular dynamics (MD) simulation method, we have seen that the use of prescribed inter-atomic potential energy functions to model the energetics and dynamics of the many-body systems under consideration lies at the very foundation of the method.

Consequently, before an MD simulation is attempted, these potentials must be constructed in advance, and they can be broken up into two-body, three-body and many-body contributions having functional forms that are devised for different types of materials. Although, there is no doubt that the classical MD simulation method, based as it is on the use of prescribed potentials, has an over coming success in the fields of condensed matter physics and materials modelling, nevertheless for problems in which several different types of atoms, or molecules, are present and hence a large set of inter-atomic potential energy parameters has to be parameterized, and in problems in which the electronic structure, and hence the bonding, pattern continuously changes during the simulation, the standard classical MD simulation, based on fixed model potentials, does not provide an adequate framework to conduct the simulation.

Ab initio molecular dynamics simulation methods are quantum-mechanical based, potential-free, methods in which the forces experienced by the atoms are computed, not from inter-atomic potentials fixed in advance, but from the electronic-structure calculations while the simulation is proceeding and the particle trajectories are unfolding in the phase space of the system under consideration. Consequently, in these methods, the focus of attention is shifted from constructing approximate potential energy functions to selecting approximate schemes to compute the many-body Schrodinger equation. The advantage of these methods therefore lies in the fact that scenarios unforeseen before the start of the simulation can develop during the simulation.

Ab initio or first-principles method is an approach to solve complex quantum many-body Schrodinger equations using numerical algorithms. The ab initio method provides a more accurate description of quantum mechanical behavior of materials properties even though the system size is currently limited to only a few hundred atoms. Current ab initio simulation methods are based on a rigorous mathematical foundation of the density functional theory (DFT). This is derived from the fact that the ground-state total electronic energy is a function of the density of the system. For practical applications, the DFT–LDA method has been implemented with a pseudo potential approximation and a plane-wave (PW) basis expansion of single-electron wave functions. These approximations reduce the electronic structure problem as a self-consistent matrix diagonalization problem. One of the popular DFT package is the Atomistix Virtual Nanolab (ATK).

4. Computation of Young’s Modulus of the SWCNT

4.1. Mechanical Property

One of the properties of CNTs is their unique strength; they are also very resilient. When CNTs are bent, they buckle like straws, but they do not break. In fact, they can easily be straightened out without any damage to the physical structure. Young's modulus is a measure of how stiff or how flexible a material is under tensile strain: how a material would react when bent or stretched.

The Young's modulus of CNTs ranges from 1.28 - 1.8 TPa (tera pascals) [3]. One tera pascal is a pressure of about seven orders of magnitude greater than atmospheric pressure. The Young's modulus of steel is 0.21 TPa, which means the Young's moduli of CNTs are typically ten times greater than that of steel. Young's modulus, Y, is the applied tensile stress over the strain:

\[
Y = \frac{\sigma}{\varepsilon}
\]  

In Equation 2, \( \sigma \) is the stress (the amount of applied force per cross-sectional area), and \( \varepsilon \) is the strain (the deformation, or change in length, caused by applied stress). The sp2 bonds can rehybridize as they are strained which make the CNTs more apt to resist breaking when strained [3].
Furthermore, the tensile strength of CNTs is $4.5 \times 10^{10}$ Pascals. The tensile strength is a measure of the amount of stress needed to pull a material apart and tensile stress is defined as a pressure, or the force per cross-sectional area, applied to the CNT. In comparison, the tensile strength of high-strength steel alloys is about $2 \times 10^9$ Pascals. CNTs are twenty times stronger than steel [3].

4.2. Calculation of Young’s Modulus for a SWCNT using an Atomistic Approach

The structural and elastic properties of SWCNTs have been computed [6] on the basis of local density approximation (LDA) to the Kohn–Sham density functional theory (DFT) [7]. The tubes studied were of the types $(6, 6), (8, 8), (10, 10), (10, 0)$ and $(8, 4)$.

In this paper, we present the calculation of Young’s modulus using ab initio atomistic approach. Performing the computations within reasonable execution times requires the selection and use of finite CNT lengths. A segment of a metallic single-wall carbon nanotube (4, 4) and semiconducting single-wall carbon nanotube (4, 0) consisting of 48 atoms is constructed as a molecule. This CNT segment will be stretched (tensile load) in this work, (as shown in figure 4) and the atomic forces and the total energy will be calculated so that eventually Young’s modulus will be calculated from the force-strain and energy-strain curves.

**Figure 4:** Stone-Wales bond stretched shown on an Armchair CNT under tension.

The atomic information of CNT (4, 4) and (4, 0) is extracted from the VNL. The unit cell of the CNT (4, 4) and (4, 0) is created by using the “Nanotube Grower” tool in the VNL. Next, the script for this unit cell is created by dropping the sample into the “Nano Language Scripter” tool. Then, the atomic positions are used in writing the script for the isolated CNT with 48 C-atoms, which consists of three of this unit cell.

Young’s Modulus ($Y$) is one of several elastic moduli. For example, bulk modulus for volume deformation, and shear modulus for surface deformation. Young’s modulus gives information about the stiffness of a material and it is defined as the Stress/Strain Ratio when Hooke’s law is valid; Young’s modulus has the unit Pascal (Pa). It can be found by calculating the slope of the force-strain or Energy-strain curve.

$$ Y = \frac{1}{V_o} \frac{\partial^2 E}{\partial \varepsilon^2} \bigg|_{\varepsilon=0} \quad (3) $$

Also, Young’s modulus ($Y$) is defined as the second derivative of the energy ($E$) with respect to the strain divided by the volume ($V$) of the tube.

4.3. A Short Survey of The Experimental Results on Young’s Modulus

Yu et al. (2000) studied the mechanical behavior of nanoropes consisting of 15 single-wall carbon nanotubes (SWCNT) [8]. Those ropes were tensile loaded inside the scanning electron microscope (SEM). An atomic force microscope (AFM) was used to apply the force on the ropes through its tip; at the same time, it was used to read the applied load. The video output of the SEM was used to record
the whole tensile-loading. After the sample was mounted inside the AFM, the tensile force applied to the SWCNT was calculated by measuring the deflection in the AFM tip for a given voltage, and that was multiplied by the force constant of the tip. As a result of this process, Young’s modulus was found to range from 0.32 to 1.47 TPa, and the average breaking strength values were from 13 to 52 GPa. The maximum breaking strain was 5.3% for this sample which is close to the theoretical value of 5% that was found by Nardelli (1998) [9].

The history of the experimental work has been started by Treacy et al. [10] when they used (TEM) and measured the thermal vibration to obtain the Young’s modulus for a multiwall carbon nanotube. They found this value to be 1.8±0.9 TPa. After that, and by using (AFM), Wong et al. [11] found this value of Young’s modulus to be 1.28±0.59 TPa and it depends on the diameter of the carbon nanotube. Later, Yu et al. [12] measured Young’s modulus between 0.27 and 0.95 TPa by using the same techniques. On the other hand,

Krishnan et al. [13] applied the method of Treacy et al. [10] on a SWCNT that has a diameter between 1.0 and 1.5 nm. They measured the mean value of the elastic modulus for this SWCNT to be of 1.25 TPa. Yakobson and his group [14] used the MD method, and found that the Young’s modulus is about 5.5 TPa. Using the ab initio methods gives more accurate values than the MD tool. Lier et al. [15] have predicted a value of higher than 1TPa for the Young’s modulus by using the ab initio method.

Another important method of calculating Young’s modulus is using the strain energy of the carbon nanotube. By computing the second derivative of the energy, Gao et al. [16] obtained the values of Young’s modulus from 0.64 to 0.67 TPa.

5. Computational Modelling of the Electrical Properties of the SWCNT

In this section, two theoretical approaches for calculating the electronic structure and the transport properties of carbon nanotubes will be described. These two methods are Density Functional Theory (DFT) and the Non-Equilibrium Green’s Function (NEGF) method. These two methods are discussed in this section. Atomistix software uses these methods to extract the electronic structure and calculate current-voltage curves for different systems. Some parameters that are used in DFT and NEGF will be discussed, and their influence on the calculations will be emphasized.

5.1. Density Functional Theory (DFT)

Different approximations derived from quantum mechanical methods are used to calculate the electronic structure for carbon nanotubes. Some methods do not treat the electron-electron interaction explicitly; two good examples are the Nearly Free Electron (NFE) model [17] and the tight-binding method [18]. Another approach is the Hartree method [17] which takes the electrostatic interaction between the electrons into consideration. This approach was extended by the Hartree-Fock methods where the exchange effects are important [17]. The system energy error remaining in the Hartree Fock approach is referred to as the “correlation energy”. The density functional theory (DFT) was created to include the correlation effects without using very costly wave function methods. W. Kohn and L. J. Sham [19] were the first investigators to formulate an efficient computational method for implementing the density functional theory (DFT), which is the basis for many atomistic-scale simulations in science. In 1998 Walter Kohn was awarded the Nobel Prize in chemistry for his development of DFT.

An essential theorem in DFT is the Hohenberg-Kohn Theorem [20] which obtains the energy as a functional of the density of the ground-state electrons. The ground-state energy is found by varying the density to obtain the minimum energy. Implementation of DFT is accomplished through the Kohn-Sham approach [19] in which a non-interacting electron reference system with an effective potential is defined and has the same eigenvalues as the multi-electron system. Solution of this single electron
Schrodinger equation yields the solution to the many-body problem; however, the effective potential in this equation depends on the electron density. Since finding the electron density requires solving for the Eigen functions, a self-consistent calculation is necessary. The accuracy of the DFT calculation depends in part on the degree of convergence of this self-consistent calculation.

The software that is used in this project employs DFT to calculate the energy, electron density and other physical properties for many-atom systems and molecules. For this work, the calculation of the total energy and the atomic forces derived from the total energy are of particular interest. The total energy consists of the sum of the kinetic energy of the non-interacting electron gas, the mean-field electrostatic energy of the electron gas and the ions, and the exchange-correlation energy of the electrons. Atomic forces are found through an analytical differentiation of the total energy terms. Exchange-correlation is treated within the Kohn-Sham DFT [20] and users can select the local density approximation [21] (LDA) or the generalized gradient approximation [22] (GGA). This software is also able to use the standard norm-conserving pseudo potentials in their non-local form [23, 24]. Minimal basis sets are selected to execute accurate calculations; for example, it uses single or multiple-zeta polarized basis sets. The use of these parameters and others is discussed in detail below. More detailed discussions of density functional theory, including the relevant equations and methods are available in the literature [25] and on the internet. A set of calculation parameters and approximations must be defined in order to use the DFT method.

5.2. Non-Equilibrium Green's Formalism (NEGF)

Non equilibrium Green’s function methods [27, 28] are usually used as a basic theory to build quantitative models for studying the transport properties in nanoscale conductors under voltage difference [29] and for quantum device simulation [30]. It is used for calculating current, effective potential and charge densities. In order for any program to simulate a quantum device, a self-consistent solution of a transport equation (5) must be performed. The calculations of the electron density and the effective potential are iterated till they converge to a self-consistent value.

A general nanodevices model is shown in figure 5. For our simulated geometries, the structure is symmetric so, the coupling parameters are equal, C1 = C2,

![Figure 5: Model of a General Nano Device](image)

The transport calculations are done when a voltage difference is applied across a channel (single-wall carbon nanotube) placed between two metallic contacts. The modification of the channel by the presence of the semi-infinite electrodes is included in “self-energy” terms in the Hamiltonian and the injection and extraction of electrons as represented by “source” and “drain” terms. To calculate the total wave function of the channel, Green’s functions are applied for the whole system (equation 4):

\[
G(E) = [E I - H - \Sigma_1 - \Sigma_2]^{-1}
\]

Here \([\Sigma_{12}]\) are defined as the self-energy matrices. These matrices describe the broadening and shift in the energy levels in the contacts due to the coupling. \([H]\) is the Hamiltonian matrix, and \([I]\) is the identity matrix. These Green functions are used in solving the Schrodinger equation to compute the self-energy matrices, “broadening” matrices, overall wave functions, and the density matrix. The transmission function \(T(E)\) is then calculated from these matrices and used to find the current density:
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\[ I = \frac{4e}{\hbar} \int_{-\infty}^{+\infty} T(E) \left[ f_1(E) - f_2(E) \right] dE \]  

(5)

In this equation, \( f_1(E) \) and \( f_2(E) \) are the Fermi functions in the source and the drain at the appropriate potentials.

5.3. Electrical Property of Single Walled Carbon Nanotubes

Carbon nanotubes possess unique electrical properties. The diameter being in the nanometer range gives rise to quantum effects. The differences in the conducting properties are caused by the molecular structure. CNTs can either be conducting or semiconducting, depending on their chirality. They are metallic if the integers of equation (1) are: \( n=m \) (the armchair structure) and \( n-m=3i \) (where \( i \) is an integer). All other structures are predicted to be semiconducting [31]. The geometry of the nanotubes determines band structures and thus the energy band gap. The energy band gap of semiconducting CNTs highly depends on the nanotube diameter and is given by:

\[ E_{\text{gap}} = \frac{2\gamma_0 d_{\text{C-C}}}{d} \]  

(6)

where \( \gamma_0 \) denotes the C-C tight binding overlap energy (2.45 eV), \( d_{\text{C-C}} \) the nearest neighbour C-C distance (~1.42 Å), and \( d \) is the diameter of a nanotube.

The conductance for carbon nanotubes is given by:

\[ G = G_0 M = \left( 2e^2 / \hbar \right) M \]  

(7)

where \( G_0 = (2e^2 / \hbar) = (12.9 \text{k}\Omega)^{-1} \) is the quantum unit of the conductance, \( e \) is electron charge, \( \hbar \) is Planck's constant, \( M \) is an apparent number of conducting channels including electron-electron coupling and inter tube coupling effects in addition to intrinsic channels [31].

5. Simulated Structures

The simulations are divided into four different sets. The first set (SET I), the simulated structures consisted of a central region of three periods (eight layers of atoms) of the armchair tubes: (4, 4); and second set (SET II) three periods (also twelve layers of atoms) of the zigzag tubes: (4, 0). The Third set (SET III) and Fourth set (SET IV), the central region are sandwiched between two carbon nanotube electrodes of the same chirality as the central region. The carbon–carbon bond lengths of the simulated (4,4) and (4,0) structures are taken as the value of 1.423 Å.

The lengths of the central regions of the simulated sections are taken as 3 periods for both tube respectively. The central region lengths of the simulated structures are 7.1 Å and 12.78 Å for both (4, 4) and (4, 0) CNTs. The simulated geometries are shown in Figure 6, 7, 8, 9. Electrode unit cells are shown by (A, B, C). The DFT-NEGF simulation parameters are selected as the following: mesh cut-off energy is 150 Ry, basis set is double zeta polarized with 0.001 Bohr radial sampling, exchange correlation functional is local density approximation (LDA) type with double zeta polarized (DZP) basis set; these parameters are chosen to provide accurate results as pointed in [30]. Brillouin zone integration parameters of electrodes are taken as (1, 1, 200), electronic temperature is 300 K, Green’s function infinitesimal is \( 10^{-5} \).

In DFT/NEGF simulations, the electrodes are assumed to be repeated infinitely in the transport direction, and to have bulk-like properties. The length of the electrodes is thus chosen to be sufficiently long to ensure that there is no interaction between the central region and the repeated images of the electrodes. The simulation box itself is also repeated in the directions transverse to the transport. The transverse dimensions of the different simulation boxes are gradually increased until no significant change in the results is observed. The basis sets used are the single-zeta polarized (SZP), and the double-zeta polarized (DZP) [32, 33]. The DZP is the most complete basis set we used, and, therefore the one that best predicts the ground state of the system [33].

The currents of CNTs are calculated using the Landauer Büttiker formula equation 8.
\[ I = \frac{4e}{h} \int_{-\infty}^{\infty} T(E) \left[ f \left( E - \mu_L \right) - f \left( E - \mu_R \right) \right] dE \]  

(8)

where \( T(E) \) is the transmission function of the CNT, \( f_L(E) \) and \( f_R(E) \) are the Fermi–Dirac distribution functions of left electrode and right electrode, respectively. The current calculation in ATK is performed using the electrochemical potentials, \( \mu_L \) and \( \mu_R \) of the left and right electrodes, respectively with the bias voltage, \( V_{\text{bias}} \) in Fermi–Dirac probability distribution functions. In our current calculations, the number of integration points of current calculation is taken as 1000 to ensure the accurate calculation of the current.

**Table 1:** The atomic information for CNT segments chiralities

<table>
<thead>
<tr>
<th>S.No</th>
<th>Chirality</th>
<th>No. of C atom</th>
<th>Radius (Å)</th>
<th>Length (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SET I (4, 4)</td>
<td>48</td>
<td>2.72</td>
<td>6.2</td>
</tr>
<tr>
<td>2</td>
<td>SET II (4, 0)</td>
<td>48</td>
<td>1.565</td>
<td>12.78</td>
</tr>
</tbody>
</table>

**Figure 6:** SET I - Isolated single walled (4, 4) Armchair carbon nanotube

**Figure 7:** SET II - Isolated single walled (4, 0) Zigzag carbon nanotube

**Figure 8:** SET III – Armchair (4, 4) CNT interconnect geometry
6. Result and Discussion
In this section, the simulated results are discussed for the four set of carbon nanotubes. First subsection discuss about the mechanical property of the SWCNT. Second subsection discuss about the electronic property of the SWCNT.

6.1. Mechanical Property
Forces and energies are calculated for the SET I and SET II carbon nanotubes. Different strains are applied to each segment to extract the strain forces and energies. These segments are stretched along the axially direction. Young’s modulus is calculated for these situations and the results are plotted (Figure 10, 11, 12, 13) and presented below in Table II.

Figure 10: SET I – The forces versus the strain curve.  
Figure 11: SET I - Total energy versus strain curve.
Figure 12: SET II - The forces versus the strain

Figure 13: SET II - Total energy versus strain

Figure 14: Young’s Modulus of the SWCNT for various Diameters
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**Force-Strain Method**

\[
Y = \frac{\text{Stress}}{\text{Strain}} = \frac{\text{Force/Area}}{\Delta L/L_0} = \frac{\text{Slope}}{A}
\]

where, Slope is the value obtained from the Force-Strain curve shown in figure 10 and 12. A is the Cross-sectional area of the CNT (Classical view). R is the CNT radius, then

\[
A = \pi R^2
\]

**Energy Strain Method**

The equation (3) rewritten as,

\[
Y = \frac{1}{L_0} \left( \frac{\partial^2 E}{\partial \varepsilon^2} \right) = \frac{1}{L_0} * \text{Slope}
\]

Where, Slope is the first derivative value obtained from the Energy-strain curve shown in figure 11, 13. \(L_0\) is the initial length of the CNT.

**Table 2:** Calculated Young’s modulus value of the SET I and SET II SWCNT

<table>
<thead>
<tr>
<th>S.No</th>
<th>Type of CNT</th>
<th>Young’s Modulus of SWCNT (TPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Force-Strain Method</td>
</tr>
<tr>
<td>1.</td>
<td>SET I</td>
<td>2.73</td>
</tr>
<tr>
<td>2.</td>
<td>SET II</td>
<td>1.80</td>
</tr>
</tbody>
</table>

According to these results, the Young’s modulus values for the SWCNT segment found by applying a first principles calculation range from 1.8 to 4.17 Tpa by using various calculation method. This is good agreement with recent experimental findings. Obviously, Young’s modulus varies significantly when using different areas. This problem is serious for the groups working in this field; thus, no agreement has been made on one value of young’s modulus for the SWCNT. Another suggested solution to avoid using the area of the carbon nanotube is to extract Young’s modulus from the strain energies by using Equation 3.

The second derivative of the total energy will be evaluated numerically and will be substituted in the equation (3) to calculate Y. The first derivative is calculated manually and plotted against the strain. The slope of this plot presents the second derivative which will be used to calculate Y. Figure 11, 13, shows the behavior of the total energy while stretching the carbon nanotube.

Young’s modulus calculated for short nanotube segments in this work is comparable to the values quoted in the journal paper for experimental and computational work on long nanotubes. According to their results, Young’s modulus for a single-wall carbon nanotube might have a value as small as 0.32 Tpa and as large as 5.5 Tpa [19]. The variation in Young’s modulus is presumably the result of using different methods and approaches. The length dependence found for the Young’s modulus of CNT segments is unexpected. As shown in Figure 14, young’s modulus of the SWCNT varies based on the chirality and diameter of the tube. By comparing these values with the ones that are calculated by using the forces, these values that are extracted from the total energies are larger by approximately 0.35 to 1.44 Tpa. The main reason for the disagreement in values is believed to reside in the sensitivity of the results to the numerical calculations of derivatives, both in the software for calculation of forces and in the manual calculations performed on the energy data. The values of Young’s modulus derived from the energy method are comparable to the values in the journal paper.

**6.2. Electrical Property of the SWCNT**

For studying and analysing the electronic properties in both types of CNTs a set of simulation have been done by using ATOMISTIX software’s. The programming and simulation are based on Density function theory, formulas and mathematical methods for solving them.
Figure 15: Bandstructure of SET I CNTs

Figure 16: Simulation result for carrier concentration of a SET I CNTs shows a uniformly distribution of electrons all over of CNT (1.08 Å$^3$)

Figure 17: Density of State of the SET I CNTs

Figure 18: Transmission Spectrum of SET I CNTs

Figure 19: Bandstructure of SET II CNTs

Figure 20: Simulation result for carrier concentration of a SET II CNTs shows a few free electron in the structure of CNT.
The electronic band structures, density of state and carrier concentration of metallic SWCNT and a semiconducting SWCNT have been studied by using the Density Function Theory. In a metallic SWCNT the sub bands do not have any gap in the energy bands and electrons spread uniformly all over of the CNT for every T, which means the Fermi level is independent of T. In metallic type the electron concentration has been estimated as $1.08 \text{ Å}^3$. In a semiconducting CNT there is a band gap in
the energy bands, sub bands overlap each other and electron concentration are very few in the structure of CNT as shown in figure 15, 16, 19, 20.

The equilibrium transport properties (no bias voltage applied) of the SWCNTs are studied firstly. The variety trend between transmission coefficient T(E,V) and the energy is plotted in Figure 18, 22. The transmission spectrum of the particular device is used to inspect the device electrode transport behaviour under various potential. The zero energy reference is taken at the Fermi level $E_F$. The system (4, 4) CNTs transmission spectrum is seen that, at the lower bias voltages 0.1V, the transmission spectrum is almost invariant to the bias voltage over the range of energy level. At higher bias voltages 1.0V, the amplitude of transmission coefficient is much lower around the Fermi level $E_F=0$. This indicates that the electron transport is much stronger at lower bias than at higher bias. This means the (4, 4) CNTs is a conductor. The system (4, 0) CNTs transmission spectrum is variable at Fermi energy level and transmission coefficient value also high at zero Fermi energy level. This means the system (4, 0) CNTs is a semiconductor and consistent with the results based on the first principle calculations.

The current–voltage (I–V) characteristics are one of the most important non-equilibrium transport properties. I–V curves of SET III and SET IV SWCNTs structures are plotted in Figure 23, 24. Since the calculation of non-equilibrium transport properties is a time-consuming work, the bias range is set from -1 to +1 V. I–V characteristics of the two different SET III and SET IV structures have a similar shape in whole bias range. The Under positive bias, the I–V curve can be divided into two parts. As the bias ranges from 0.0–1.5V and 1.5–2.0 V, the current will be strengthened by the increase of the bias voltage. While the bias is among 0.8–1.5 V, NDR effect is observed. The transport properties of the isolated semiconductor CNT is that when the voltage is lower than 1.4V reported in [34], there is no current following through the CNT, which is an obvious sign of semiconductors. Great difference is presented in the transport properties between the isolated (4, 0) and CNT-CNT-CNT interconnect device. The voltage is lower than 1.5V, the current through the CNT–CNT–CNT system increases linearly with the increasing voltage. Once the voltage is higher than 1.5V, the corresponding current tends to be saturated.

From Equation 8, the magnitude of current is determined by the transmission spectrum and the energy range, in which the integration is realized (named as bias window). The increase of the bias window means that more molecular orbitals contribute to the formation of the current.

7. Conclusion
A good deal of effort has been focused on obtaining estimates of the values of the Young’s modulus of the nanotubes. Estimates obtained depended on the theoretical models or the inter-atomic potentials used. For SWCNTs, computed values ranging from 0.8 to 4.17 TPa have been reported, seems to be the accepted result. Experimental values of Young’s modulus for SWCNTs tend to support the computed values at the lower end of the range, i.e. around 0.37–5.55 TPa. For various chirality of nanotubes, the computed estimate of the Young’s modulus has given a value around 0.8 – 4.17 TPa. It is, therefore, clear that estimates obtained, although they are of the same order of magnitude, differ substantially from one study to the next. Even ab initio computations have not been able to provide an estimate comparable to the experimental results, giving values in the range of 0.5–4.8 TPa depending on the thickness adopted for the tube. Clearly, this aspect of mechanical properties continues to pose a challenge to computational research.

In summary, the method in combination of DFT with NEGF, the transport properties of the (4, 4) and (4, 0) CNT interconnected geometry are calculated. The results show that the coupling effect plays an important role in the transport properties, a conductance plateau is found in the transmission spectra near the Fermi energy, the I –V curve can be divided into two parts: the current increases linearly with the voltage within the range of 0.0–1.5V and trends to be saturated in the range of greater than 1.5V. Our results are helpful to study the working principles of the CNT electronic devices and design new ones.
Carbon nanotubes often exhibit defects such as pentagons, heptagons, vacancies, or dopants that drastically modify their electronic properties. The electronic properties of defective nanotube-based structures are, of course, more complex than those for infinitely long, perfect nanotubes. The introduction of defects into the carbon network is thus an interesting way to tailor its intrinsic properties to create new potential nanodevices and to propose new potential applications for nanotubes in nano-electronics. Because carbon nanotubes are metals or semiconductors, depending sensitively on their geometrical structures, they can be used to form metal-semiconductor, semiconductor-semiconductor, or metal-metal junctions. These junctions have great potential for applications because they are of nanoscale dimensions and are made entirely of a single chemical element. Nanotube junctions thus can behave as nanoscale metal-metal junctions, metal-semiconductor Schottky barrier junctions, or semiconductor intra molecular junctions with novel properties and these different types of junctions can serve as building blocks for nanoscale electronic devices.

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**References**


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