Environmental Friendly Device: Modeling of Carbon Nanotube with Optimum Chirality

Soheli Farhana and AHM Zahirul Alam

Department of Electrical and Computer Engineering, Faculty of Engineering, International Islamic University Malaysia, 53100 Kuala Lumpur, Malaysia.

Abstract: An optimum chirality of carbon nanotube (CNT) is modeled and analyzed in this paper. CNT is a tubular form which is made from a graphene sheet. Thus only graphene can be contributed through its' electronic properties to setup an optimum CNT. Therefore, First we describe the geometrical structure calculation and then analyzed the graphene electronic structure and thus this graphene surface forms a nanotube. Theses electronic properties are designed from tight binding (TB) model for graphene. Furthermore, geometrical calculation shows that misalignment and pyramidization angle with chirality (25,0) which is semiconducting zigzag for SWCNT and MWCNT. Finally the minimum value of CNT bandgap of 0.4401eV shows that the optimum chirality is (25,0) for the modeling of carbon nanotube.

Keywords: CNT, chirality, TB.

INTRODUCTION

Carbon nanotube (CNT) is a rolled graphene sheet is single-walled (SWCNT) or multi-walled (MWCNT) structures (Kaiser et al., 2007). CNT geometric structure makes it either metals or semiconductors (Qin, 2000). Copper current density can be reached less than 1000 times smaller than axial current density (Hersam et al., 2008). The axial mobilities are $\mu_a = 150 \text{ cm}^2/\text{Vs}$ and $\mu_h = 220 \text{ cm}^2/\text{Vs}$, also semiconductor CNT has small band gap rather not to have band gap of metal CNT (Baughman et al., 2002). Due to small band gap and diameter of semiconductor CNT, it presents the Aharonov-Bohm effect at room temperature (Ijäs and Harju, 2012). CNTs have 300 times higher tensile strength than carbon steel due to their perfect mechanical characteristics (Tasis, 2006). With a better thermal conductance CNTs are claimed as a stable material than the other materials considering for electronics device fabrication (Ghosh, 2010). Thus CNTs are used to be applied for nanoelectronics applications. Furthermore CNTs present a tough electronic resonance (Han et al., 2011). The CNT resonance is used to manufacturing of very high frequency electronics device such as sensors, transistors etc (Wei, 2012) by applying the suitable current values and the doping conditions. Therefore CNT manufactured transistors with every electron perform well in room temperature (Thelander et al., 2003). Finally, CNTs equipped devices are exhibits higher performances in various applications and produced itself as good marketable materials due to their low cost, electrical and mechanical properties (Sire et al., 2012; Sun et al., 2011; Hecht et al., 2011). Though several CNTs are investigated using different chirality (Nasibulin et al., 2011), but still there are some current leakage is found due to their higher band gap.

In this paper, we focus on the investigation of molecular atomic structure of CNTs and geometrical calculation of CNTs. These geometrical calculations enable to analysis modeling of carbon nanotube with better chirality, which is zigzag semiconduction which will exhibit a small band gap.

Carbon Nanotube Structure:

Carbon nanotube characterization is done by its chirality which exists with its' length and a vector called the chiral vector. Chiral vector is the sum of the multipliers of the two base vectors, like equation (1).

$$C_h = ma_1 + na_2$$  \hspace{1cm} (1)

This chiral vector can be mentioned by $(m,n)$ and $a_1$ and $a_2$ are the unit vectors of the graphene cell is shown in Fig. 1. To obtain the tube from a graphite sheet we can roll the sheet in a way that this vector be put on the circumference $C_h$ of the tube and thus the perimeter of the tube will be equal to the length of the chiral vector.

From the equation (2), a second vector called the Transitional vector which denote by $T$.

$$T = t_1 * a_1 + t_2 * a_2$$ \hspace{1cm} (2)

This vector $T$ is perpendicular to the chiral vector $C_h$. If we define a base point and place $C_h$ and the $T$ vectors on that, then $T$ is the shortest site vector perpendicular to $C_h$. A nanotube unit cell is obtained from rolling
the part of graphitic sheet enclosed by the rectangle resulting from T, C_h as shown in Figure 1, a nanotube graphene cell shown in the shaded area.

Fig. 1: Graphene sheet with CNT unit cell.

To more precisely obtain the T vector we can derive it from the m, n components of the C_h vector. If we show the components of T with t_1 and t_2, as T is perpendicular to the C_h, the inner product of these vectors is equal to zero and we can conclude equation (3).

\[ t_1 \cdot a_1 + t_2 \cdot a_2 = 0 \]  \hspace{1cm} (3)

The shortest vector \( t_1 \) and \( t_2 \) that are valid according to equation 2 we can divide \( t_1 \) and \( t_2 \) by their greatest common divisor or in short form greatest common divisor (gcd), to obtain the shortest atomic site vector in the direction, perpendicular to the C_h vector.

\[ d_R \] as in equation 3, we can find \( t_1, t_2 \) as shown in equation (5) and equation (6).

\[ d_R = \text{gcd} \left( 2m + n, 2n + m \right) \]  \hspace{1cm} (4)

\[ t_1 = \frac{2m+n}{d_R} \]  \hspace{1cm} (5)

\[ t_2 = \frac{2n+m}{d_R} \]  \hspace{1cm} (6)

Chiral angle is found here in between the chiral vector and the a1 base vector. The twist angle or the helix angle and is denoted by \( \theta_c \) and can be obtained using inner product of C_h and a_1 as shown in equation (7).

\[ \theta_c = \arctan \left( \frac{\sqrt{3}m}{2n+m} \right) \]  \hspace{1cm} (7)

The diameter of the tube can be computed using the equality of the length of the C_h and the nanotube’s circumference, and finally we can obtain the diameter using equation (8).

\[ d_{\text{cnt}} = |a_1| \frac{\sqrt{n^2 + nm + m^2}}{\pi} \]  \hspace{1cm} (8)

If the C_h is defined as \( (n, 0) \) it is given the name zigzag nanotube and if the C_h is defined as \( (n, n) \) then the tube is called armchair and these refer to the form shaped on the circumference of the tube.
Tube Structure:
A graphene is a single layer sheet from a many layer form of graphite. This single layered graphene sheet will then form a CNT. CNTs are bonded in a hexagonal blueprint of graphene layer. CNTs are looking as a tube structure. CNT can be single walled nanotubes (SWNT), as if a single sheet had been rolled up, or multiwalled (MWNT), similar in appearance to a number of sheets rolled together. A single walled nanotube diagram is shown in Fig. 2.

![Diagram of a Single Walled Nanotube.](image)

Also a multi-walled nanotube diagram is shown in Fig. 3.

![Schematic models for Multi-walled Nanotube.](image)

Single-wall carbon nanotubes (SWCNTs) are constructed of one single carbon layer. 0.4nm up to 3 nm is the distinctive diameter of SWCNT. Multi-walled carbon nanotubes (MWCNTs) are occupied with a number of coaxial carbon layers with a distinctive diameter of 2nm up to 100 nm.

A \((n, 0)\) SWCNT is called zigzag nanotube and a \((n, n)\) SWCNT is called armchair nanotubes, where chiral nanotubes are made of integers \((n, m)\). Different structured SWCNTs are shown in Fig. 4.

![Different Structure: (a) Zigzag SWCNT; (b) Armchair SWCNT; (c) Chiral SWCNT.](image)

MATERIALS AND METHODS

DFT Optimized Diameter:
Circumferential vector is \(\hat{C} = (0, C)\) and it makes an angle with the reference \(x-y\) axis. The bond vectors are presented in the new coordinate system by using a rotation of the axes:
\[ \hat{r}_1 = a(0,1) \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix} = a(-\sin x, \cos x) \]

\[ \hat{r}_2 = \frac{a}{2} \begin{pmatrix} \sqrt{3} & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix} = \frac{a}{2} (\sqrt{3} \cos x - \sin x, \sqrt{3} \sin x + \cos x) \]

(9)

\[ \hat{r}_3 = \frac{a}{2} (\sqrt{3}, 1) \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix} = \frac{a}{2} (\sqrt{3} \cos x - \sin x, \sqrt{3} \sin x + \cos x) \]

Structure of Carbon Nanotube:
Pyramidalization angle (\( \Phi_{pgr} \)) is determined by summing two angles getting from carbon atoms. After that 180° is subtracted and then divided by 2. This gives 2.3° for the set of carbon atoms for a (25,0) SWNT.

RESULTS AND DISCUSSIONS

The analysis of the electronic properties of a larger number of different carbon nanotubes (Farhana et al., 2013) in the diameter region of 0.3 to 1.95 nm focusing on the larger diameter with small diameter and including semiconducting tubes (zigzag; 25,0) using molecular theories and geometrical properties is shown in Table 1. To summarize the results obtained so far, simulation shows the lower band-gap of 0.4401eV is obtained from (25, 0) chirality semiconductor type CNT. Table 2 made a comparison with several works to verify the lower band-gap.

Table 1: Analysis different chirality of CNT parameters.

<table>
<thead>
<tr>
<th>n</th>
<th>m</th>
<th>( d_{DFT} ) (nm)</th>
<th>( r_1 ) (Å)</th>
<th>( r_2 ) (Å)</th>
<th>( r_3 ) (Å)</th>
<th>( \Phi_{pgr} ) (°)</th>
<th>( E_g ) (eV)</th>
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<td>1.411</td>
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</table>

Geometrical parameters from Table 1 are stated as follows: 

n, m: chiral indices, \( d_{DFT} \) (nm): optimized diameter, \( r_1 \) (Å), \( r_2 \) (Å), \( r_3 \) (Å): bond lengths misalignment angles, \( \Phi_{pgr} \) (°): pyramidization angle, and \( E_g \) (eV): Band gap.

Furthermore, table 1 shows the simulated data for zigzag CNT for number of atom versus diameter for zigzag tube.

Table 2: Comparison of Band Gaps for Carbon Nanotubes.

<table>
<thead>
<tr>
<th>n</th>
<th>m</th>
<th>( d ) (nm)</th>
<th>( E_g ) (eV)</th>
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<tr>
<td>25</td>
<td>0</td>
<td>1.9510</td>
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</table>
Conclusions:

We have described geometrical calculation with pyramidization angle and band gap for the selection of optimum CNT. Analysis of this calculation is necessary for appreciating technology potential of new CNT device.

REFERENCES


