Small Band-gap-based CNT for Modeling of Nano Sensor

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Abstract

Modeling phenomena of small band-gap Carbon Nanotube (CNT) is analyzed in this paper. Device physics of CNT is studied and do the calculation of sub-band for zigzag CNT to model small band-gap tubes. Each carbon nanotube is illustrated as a single graphite sheet turned round into a cylindrical shape so that the arrangement is one dimensional with axial proportion. A comparison is made with the current literature to show that the proposed chirality CNT with small band-gap which performs the modeling of nano sensor. Furthermore, a sensing device is modeled and discussed in this paper. This carbon nanotube based sensing device makes it possible produce huge amount of nano chips as a disposable cartridge for diagnostic purposes. The optimum CNT is proposed in this paper to model a nano-electrode device. This research outcome shows that the importance of identification with verified uniqueness of high reliability and economical micro-fabrication for cost effectiveness.

Keywords: Nano sensor; nanotube; graphene; bandgap.

1. Introduction

The stable diminution in the size of transistors on integrated circuits according to Moore’s law is realized in the semiconductor industries. The channel length is reduced to increase the speed of operation and the number of components per chip, the short-channel effects, tunneling effect (due to too thin gate insulation), interconnects problems etc. So it is not possible to reduce the size further to produce nano device. Hence now it is necessary to adopt new material or technology which preserves a lot of what’s good about the number of remarkable electrical as well as properties of semiconducting Carbon Nanotubes (CNTs) that are superior for electronic devices. CNTs are
members of the carbon family of fullerenes that was discovered almost two decades ago [1]. From the day of carbon discovery and their derivative have been considerable attention given to these macro molecules. However, even though the interest and effort of the scientific community in the research of carbon nanotubes are considerable [2], some of the basic properties such as optical, magnetic, and magneto-optical properties are still not well understood. Lower diameter with higher band-gap makes CNTFET for electronic device application. This research mainly focus on the semiconducting property of CNTs as electrical properties such as diameter, energy gap for nano device production. Nano device production and marketing is very difficult in terms of the price and dimension of the device [3]. In engineering perspective, carbon electrodes have shown similar characteristics with the carbon nanotubes. Such as faster transport, huge potential and compatible with biological substances are the main characteristics. Very rare material contains these characteristics which is essential for amplifying the wave getting from the objects. Therefore, a metal electrode of platinum can be electrolyzed water before reaching the electro-potential required for the analysis of many biological substances. That's why huge amount of current produce to distort the real wave. By replacing electrode to carbon will overcome this limitation to get a better performance from the sensing device. A carbon nanotube (CNT) is shown in Fig. 1 to enable this research for modeling a sensing device.

This paper's is organized as follows. Electrical properties of carbon nanotubes are shown in section 2. After that a brief analysis is presented in section 3. Modeling of CNT devices is explained and shown in section 4. Finally section 5 presents results and discussion of the CNT sensing device.

2. Carbon Nanotubes

For the significant electronics properties of CNTs, it becomes top position nano-material in the field of nano technology. Therefore, CNTs are recognized to fit for the nano-electronic FETs since they have their distinctive electromechanical and thermal properties. Single walled and multi walled CNTs are considered for the nanotechnology research. These two types of CNTs are useful for their different characteristics in device construction [6]. A complete study of CNT electronics structure was analyzed [7-9]. A CNT is a nano-scale substance with very small radius as 1.95nm [10-17]. Based on configuration of CNT, it is rolled up tube like graphene sheet. By considering single walled CNT is identified by its chirality (n,m) where n and m are index numbers in the single graphite network. Metallic CNT is considered by (n-m)/3, on the other hand others are semiconducting CNT.

2.1. Reciprocal lattice

The primal cell of a CNT is described from the unit vectors,

\[ R_1 = \frac{a}{2} \left( \sqrt{3} \hat{x} + \hat{y} \right), R_2 = \frac{a}{2} \left( \sqrt{3} \hat{x} - \hat{y} \right) \]  

where, \( R_1 \) and \( R_2 \) are the unit cell vectors of a CNT and \( a = 2.49 \) Å.

2.2. Energy Dispersion Relation

Nanotubes’ K relations need to derive due to examine the conductivity properties of the nanotube. The equivalent relation of a two dimensional graphene lattice may solve this requirement. Graphene electronic structure helps to calculate the energy dispersion for CNTs,

\[ E_{2D}(K) = \pm V_{ppr} \left\{ 3 + 2\cos(KR_1) + 2\cos(KR_2) + 2\cos[K(R_1 - R_2)] \right\}^{\frac{1}{2}} \]  

where \( V_{ppr} \), is the adjacent shift integral. The 3D view of energy dispersion relation is shown Fig. 2.
Fig. 1. Zigzag open end nanotube with diameter of 1.95nm

Fig. 2. Energy dispersion relation between valence and conduction band
Single-walled CNTs’ 1D energy band calculation can be done as [3]:

\[
E_{1D}(K) = \pm V_{pp} \left[ 1 + 4 \cos \left( \frac{\sqrt{3}K_x}{2} a \right) \cos \left( \frac{K_y}{2} \right) + 4 \cos^2 \left( \frac{K_y}{2} \right) \right]^{1/2}
\]

(3)

Here, \(K_x\) and \(K_y\) are the wave vectors. The potential application of CNT can be seen in the electronics market.

3. CNT Analysis

3.1. Zone Folding

3.1.1. Armchair tubes

Simple zone folding predicts that if the difference of the \(n, m\): chiral indices is divisible by 3, then the \((n, m)\) nanotube is metallic. We shall refer to these nanotubes as "zone folding metallic", or shortly, ZF-M tubes.

Using the following equations to obtain calculate different nanotube. The tube diameter is then given by,

\[
d_t = \frac{L}{\pi} = \frac{a}{\pi} \sqrt{n^2 + nm + m^2}
\]

(4)

The bandgap is given by,

\[
E_g = 2\gamma_0 a_{cc} / d_t, d = \gcd(n, m)
\]

(5)

if \((n-m)\) is divisible by 3 then \(d_t=3d\) otherwise, \(d_t=d\).

\[
N_{at} = \frac{n^2 + m^2 + nm}{d_t}
\]

(6)

3.1.2. Zigzag tubes (Semiconducting tubes with bandgap)

Simple zone folding predicts that if the difference of the \(n, m\): chiral indices is not divisible by 3, then the \((n, m)\) nanotube is a semiconductor with a well-defined, often referred to in the literature as primary band gap. We shall refer to these nanotubes as "zone folding semiconducting", or shortly, ZF-S tubes.

3.2. Sub-Bands Calculation, \(\Delta p\)

The minima energy of the CNT sub-bands is given by,

\[
E(k_1,k_2) = \pm V_{pp} \pi \sqrt{1 + 2 \cos(2\pi k_1) + 2 \cos(2\pi k_2) + 2 \cos(2\pi (k_1 - k_2))}
\]

where \(k_1\) and \(k_2\) depend on the \(n\) and \(m\) parameters,

\[
k_1 = \frac{q}{N} \left( \frac{2n + m}{d_R} \right),
\]

\[
k_2 = \frac{q}{N} \left( \frac{2m + n}{d_R} \right)
\]

(7)
Hence, the values of $E(k_1,k_2)$ are successively calculated using (10). Then, the lowest values are ordered to select the minima of the first, second, ...., $p$th energy sub-bands, $1, 2, \ldots, p$ is shown in Fig. 3.

From the analysis of zigzag CNT (25, 0), the energy of each of the sub-band properties ranging from $1.487233, 1.129917, 0.744495, 0.416031, 0.513978, 0.94504$ and $1.433064$ for 1 to 7 numbers of sub-band focusing on the smaller energy band including semiconducting tube. From the above energy of the sub-band, $0.416031$ is the lowest energy dispersion for (25, 0) CNT.

Generally metals are used in constructing electrodes. A perfect electrode should have application required conduction, appropriate dimensions, prototyping simplicity, reliable characteristics, environmental friendly and compatible, performances of signal properties, electromechanical properties, functional integrated system for the better performances. Therefore, carbon nanotube can be the replacement of metals for constructing small scale electrode for the various application.

4. Modeling of Nano Device using CNT

4.1. Nano Device in CNT Electronic Structure

The use of CNT is increasing everyday for various field of implementation. CNTs are also contributed in medicine application industry [4]. To consider in advance technology in electronics, CNT has a great contribution towards the human society by creating a green technological concept. Where CNTs made devices are easy to recycle to prevent the environment from the pollution. Nano Electro Mechanical System is one of the major invention in this century where CNT play an important role for the massive production. This Nano Electro Mechanical System device will enable to carry-out the sensing experiment. The smaller energy band-gap produce a semiconductor device using the CNT [5]. Biological medical field is very broad to conduct research on sensing devices. It will be in nano to micro scale for the sensing space for the development of this device. A CNT electrode named nano-electrode can be performed to build a sensing device in this NEMS field of research. A expected CNT sensing device operation is shown in Fig. 5. CNT electrode is acting here as the end effector of the device activated with the investigate substances. The resistance of Single walled CNT equivalent circuit is shown in Fig. 4. Due to spin degeneracy and sub lattice degeneracy of electrons in graphene, each nanotube has four conducting channels in parallel. Hence the conductance of a single ballistic single-walled CNT (SWNT) assuming perfect contacts. This is the fundamental resistance associated with a SWCNT, this fundamental resistance is equally divided between the two contacts on either side of the nanotube.
4.2. Nano-electrode in Sensing Application

Signal to Noise Ratio (SNR) is the measurement method for sensitivity of an electrode. The flowing current create noise for the capacitive properties involvement at the electrode is shown as see Fig. 5:

\[ i_n \propto C_d^0 A \] (9)

The capacitance is denoted by \( C_d^0 \). By reducing the electrode size to 20 nm from 20 \( \mu \)m, the SNR would be modified in 1000 times.

Electrode dimension refers to the function of the electrode's response time.

\[ \tau = R_c C_d = r C_d^0 / 4k \] (10)

where electrolyte conductivity is denoted by k. The applied properties of this system would be more faster once the size reduced nanometers [7]. Therefore, the sensitivity can be radically developed by decreasing the dimension of the electrodes to nano-size.

5. Results And Discussions

5.1. Optimum CNT

The analysis of the sub-band properties of a larger number of different carbon nanotubes 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 is shown in Table 1. To summarize the results obtained so far, calculation shows the lower band-gap is obtained from (25, 0) chirality semiconductor type CNT, which can be able to contribute for building faster switching CNTFET.

Table 1 made a comparison with several works to verify the lower band-gap.
5.2. CNT Experimental Result for Nano-device

As a first step for developing an electronic CNT device, a small band gap device was successfully designed and characterized using Scanning electron microscopy (SEM) due to size, electrical properties, improving sensitivity, response, and recovery times. It also induces carrier-scattering at the SWCNT junctions, and decreases the resistance. We developed a technique to image the long nanotubes using an SEM. SEM images were taken at low acceleration voltage (10 kV) and the SEM is switched to low magnification mode.

SWCNTs are arranged in a forest configuration as shown in Fig. 6(a). 300°C are required to produce the CNT. Fig. 6(a) shows an experimental image of CNT bundles which have been conducted in characterization laboratory. With a nominal diameter of 1.95nm, lengths of 5nm-15μm of the single walled CNT forests are created smooth structure. The top and perspective view of the CNT bundles electrode is in Fig. 6(b) by SEM.

![Fig. 6. (a) Scanning electron microscopy (SEM) images of CNT (b) SEM for CNT bundles](image-url)
6. Conclusions

It can be concluded that the semiconducting property of carbon nanotubes can be achieved provided that the chiral vector (n-m) is not divisible by 3. The band gap of the CNTs can be reduced by increasing the value of n of chiral vector. Therefore, high speed CNTFETs can be designed with (25,0) chiral vector due to its small band-gap. Therefore it may represent a new paradigm for devices in the 21st century. An analysis is conducted to model a nano scale electrode for sensing device in this work. CNT used here for the modeling of the electrode. CNTs are successfully applied the transfer technology to setup electrode with a nominal diameter of 1.95 nm. This model will reduce the error rate of biosensor device measurement.

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References