Journal of Basic and Applied Engineering Research
p-ISSN: 2350-0077; e-ISSN: 2350-0255; Volume 5, Issue 3; January-March, 2018, pp. 208-211

http://www.krishisanskriti.org/Publication.html

Nanotechnology and Electronic Transport through Bent Carbon Nanotubes, Theoretically

Dr. Ali Ahmad Ansari

Asistant Professor of Physics, MKCET, Veriadangi, Kishanganj, Bihar, India
E-mail: aliahmadansari456@gmail.com

Abstract—*The present paper reports the theoretical study of nanotechnology and electronic transport through bent carbon nanotubes in usual manner. The bending phenomena in carbon nanotubes have been study experimentally and had indicated that under sever bending the buckling is usual way for nanotubes to reduce strain. The usual approach to the theoretical modeling of buckling phenomena has so far made use of classical potential. Even for calculation of the electronic properties of the bent tubes, which make use of relatively more sophisticated quantum tight binding Hamiltonian, the scattering geometry of the bent nanotubes has been obtained using classical potential. The relaxed procedure based on classical potential does not take into account the increased σ-π hybridization as a result of bending, especially at larger bending angles. However the increased hybridization is expected to have a decisive effect not only to electronic structure but also on the force and relaxed atomic configuration themselves. The inter relation of electronic and mechanical properties of carbon nanotubes give rise to natural speculation for possible application. It has been shown both experimentally and theoretically that the reversible bending of nanotubes can be used to alter their conduction which in turn may be used in nano electromechanical switch and sensor application. Previous calculation of nanotubes young modulus empirical force constant and Ab-inito models indicate that it is independent of chirality of the tube. However for larger strain, it had shown that the most of the axial strain is borne by the bonds, parallel to the tube axis. We will use Amir A Farangian and Bons techniques for purpose of research work. We will choose four orbital per atom tight binding approach for the parameterization for carbon both to obtain optimized geometries and to calculate the electronic properties.*
We will study electronic transport through bent carbon nanotubes and will establish a correspondence between the mechanical deformations and current that is passing across the deformed region. The theoretical obtained result will be compared with previous obtained theoretical and experimental result.

Keywords*: Nanotechnology, carbon nanotubes, 4-orbital tight binding approach.*

1. INTRODUCTION

Nanotechnology-

Nanotechnology is a field of applied science and technology covering abroad range of topics.

The main unifying theme is the control of matter on a scale smaller than one micrometer as well as the well as the fabrication of devices on this same scale. It is a highly multidisciplinary field, drawing from same fields such as colloidal science, device physics, and supramolecular chemistry. Much speculation exists as to what new science and technology might result from these lines of research [1].

Nanotechnology and nano science got started in the early 1980s with two major developments; the birth of cluster science and invention of scanning tunneling microscope (STM).

This development led to discovery of fullerenes in 1985 and carbon annotates a few years later. Carbon nanotubes have recent received extensive attention due to their nanoscale dimension and outstanding materials properties such as ballistic electronic conduction, immunity from electro migration effects at high current densities, and transparent conduction [2].

As nano tube fabricated it bends automatically due to its nano shape. Bending of nanotube provides buckling and this bucking is usual way for nanotube to reduce its strain. After that relaxed configuration is obtained. Now nano tube is ready for various purpuses. [3].

Classification of carbon nanotubes

(a)Based on conductivity: (1)Metallic

(2)semiconducting (b)Based on chirality

(1)Zig-Zag

(2)Armchair

(3)Chiral

(c)Based on layers

(1)Single walled nanotubes(SWNT)

(2)Multi walled nanotubes(MWNT)

1. Classification based on conductivity;

The conductance of carbon nanotube is mainly affected by its chirality(amount of twist in the tube).Twisting is found to transform the metallic nanotube to a semiconducting one with a bandgap that varies with the twist angle as shown in fig.1.

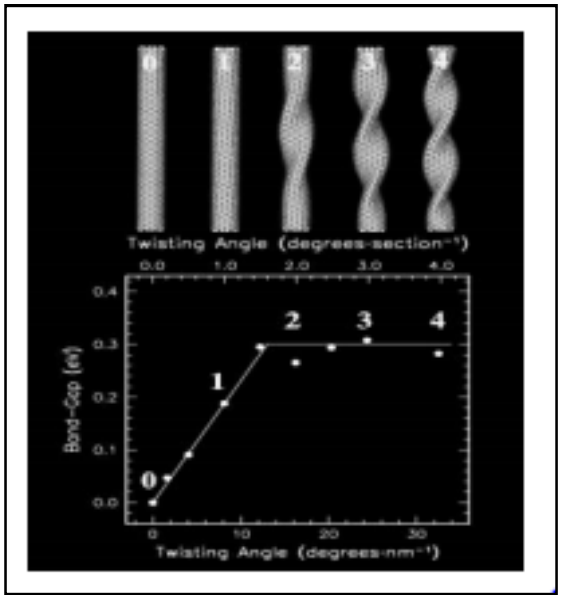

Figure no. 1

2. Classification based on chirality;

CNTs based on their chirality are classified as zig-zag armchair and chiral. Nanotubes form different types, which can be described by the chiral vector (n,m), where n and m are integers of the vector equation. Nanotubes based on chirality is shown in fig.2.

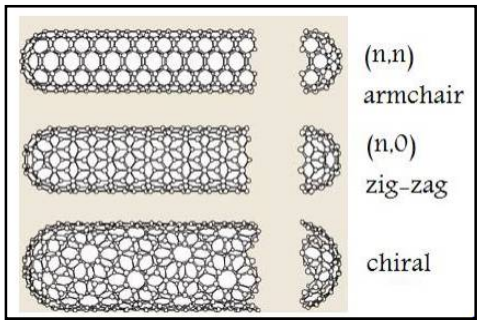

Figure no. 2

3. Classification based on layers;

Carbon nanotubes are an outgrowth of the formation of carbonfullerences, such as C60 bucky ball molecules. There are two basic types of nanotubes. Single walled nanotubes (SWNTs) have one shell of carbon atoms in a hexagonal arrangement as shon in fig.3. Multiwalled nanotubes (MWNTs) consist of multiple concentrically nested carbon tubes as shown in fig.4.

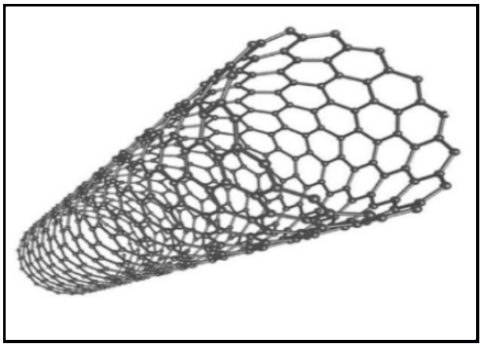

Figure no. 3

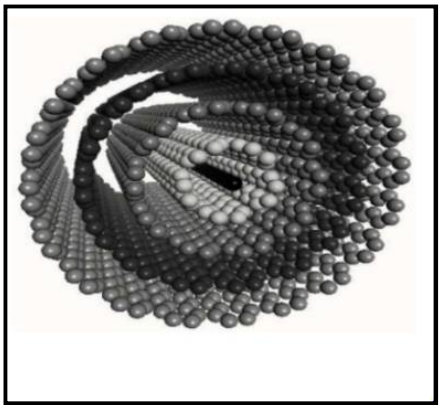

Figure no. 4

2. INTRODUCTION OF RESEARCH WORK-

When a graphene sheet of one atom thick can be rolled into a tube then obtained helical tube is called bent carbon nanotube. The radii of this tube be less than one nanometer and its diameter be 1.4nm. As nanotube is fabricated it bends automatically due to its nanoshape. Bending of nanotube provides buckling and this buckling is usual way for nanotube to reduce its strain. After that relaxed configuration is obtained. Now nanotube is ready for various purposes in nanotechnology. The bending of grapheme continuous attracts the great interest on the basis of theoretical and experimental point of view[5].The relation between mechanical and electrical properties of nanotube provides useful base for theoretical investigation as well as practical applications. It has been shown by both experimentally and theoretically that reversible bending of nanotube can be used to alter their conduction which turn may be used in nano electromechanical switch and sensor application. Here we study electronic transport through bent carbon nanotube and establish the relation between mechanical deformation and current passes through deformed region. First we obtain possible configuration of BCNT structure using four orbital per atom tight binding model. Next conductance characteristics of relaxed structure are derived. After that we calculate the current, passes through the nanotube. Finally we focus on bending angle and current-voltage characteristics (I-V, characteristics).

3. RESULTS AND DISCUSSION

MODEL AND METHODS

In order to obtain relaxed structure under bending and to calculate transport property, there are three nanotubes have been Considered in this study. These tubes are armchair, zig-zag and zig - zag arm chair kink structure. Considering large no- of atoms in this system; using classical potentials. [7].We choose 4- orbital per atom tight binding approach for, parameterization of carbon, both to obtain possible geometry and to calculate electronic transport properties of BCNT.[8].

4. TECHNOLOGY AND METHODOLOGY

In order to obtain the successes bending angle in graphene Sheet. We have fixed eight carbon rings at each end of nano tube (96 atoms for armchair and 80 atoms for zig - zag). The structure is minimized such that, the maximum force acting on each free atom (unconstrained atom) becomes less than 0.05ev. Now relaxed configuration is obtained for different bending angles. Now we focus on transport properties and calculate the conductance. Conductance is calculate by the formula.

$$G(E,V) = \left(\frac{2e^2}{h}\right) T(E,V)\ldots. \quad \text{(I)}$$

After that I(v) characteristics is obtained by the using Landauer Buttiker formula[13]

$$I(V) = \frac{2e}{h} \int dET\ (E,V)\ [f_B\ (E - \mu_B) - f_A\ (E - \mu_A)\ ] \quad \text{(ii)}$$

Where a bias voltage is applied to the bent region. The chemical potential of two leads µA &; µ B are assumed to be pinned at V/2 to – v/2. This determines the shift of band structure & density states of leads. [9].

Mechanical response of nanotube

The results of obtained geometry are shown in fig. 5. Compare the result shown in fig.5. with previous obtained structure using classical potential for carbon nanotube structure. We find that an overall extension of bent region in tight binding result as compared to the classical result. This is including that the increased σ-π hybridisation within the tight binding model especially at larger bending angle [10,11].

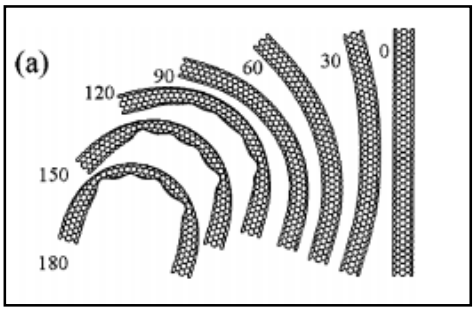

Figure no. 5

Conductance characteristics of nanotube

Here we calculate the conductance characteristics of relaxed bent structure of nanotube at zero bias. After that these are calculated at different carrier energies. Here we assumed that two semi infinite perfect tubes to be attached to the two ends of the bent region. This is shown in fig. 6. This fig. Illustrates the conductance results for bent region of bent carbon nanotubes [12].

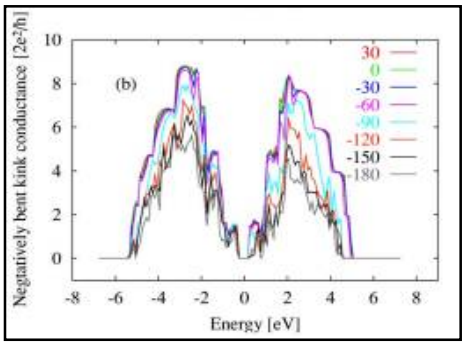

Figure no. 6

Current voltage [I-V] characteristics of nanotube

In this context it is found that the bending angle increases the current passing through the bent arm chair nanotube decreases while that of zig-zag tube increases. It is found that the conduction of bent tube under bias is determined by the number of conducting channels available within the two semi infinite leads and corresponding transmission co-efficient between any pair of them. The I-V characteristics of bent structure is shown in fig.7. Here we consider carbon nanotube with pseudo gap of 3 eV.

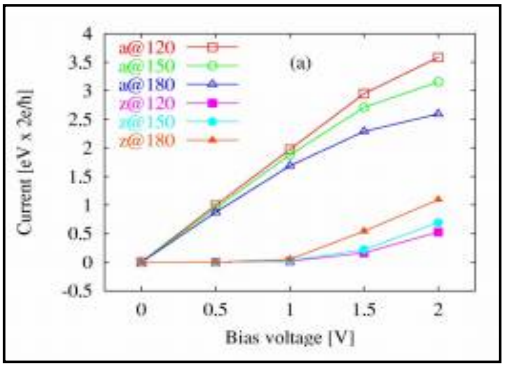

Figure no. 7

5. CONCLUSION

In summary we have calculated the relaxed configuration of nanotubes at different bending angles.

Mechanical properties of nano tubes at larger bending angles are observed. We found bands parallel to zig- zig tubes axes.

When applied voltage be zero then Conductance of all the tubes be zero, but on non zero voltage conductance be differ.

At larger bending angles, current passes through metallic structure decreases where as in semiconductor increases.

The relation between mechanical response and electronic transport of nano tube can be used to nano electromechanical switch and nano electromechanical sensors application & design.

6. FUTURE SCOPE OF WORK

It has been shown both by theoretically & experimentally that the reversible bending of nano tube can be used to alter their conduction which in turns may be used in nano electro mechanical switch & sensor application

7. ACKNOWLEDGEMENT

I am indebted and grateful to my supervisor Dr. Amita Sharma, Associate Professor, Deptt. of Physics, B.R.A.B.U. Muzaffarpur Bihar for her constant guidance and encouragements for research work.

My thanks to Dr. B. Rai Prof. and Head Univ. Deptt. of physics B.R.A.B.U. muzaffarpur.

My thanks are also due to Dr. V.K. Thakur Prof. and Former Head, Dr. Madan Jee Professor and former Head University Deptt. of Physics, B.R.A.B.U., Muzaffarpur. Dr. R.B. Chaudhary, Dr. L.K. Jha, Dr. S.N. Chatterjee, Dr. Bhagwan Prasad for encouragement and suggestions for research work.

I am also obliged to Dr. B. Roy, Dr Nashim Ahmad, Dr. Suresh Chand and other faculty members for valuable suggestion for research work.

REFERENCE

[1] Carbon nanotubes – seminar reported by Shuhab – U - Tariq – 1SIO3EC109(2007)
[2] AC-2007-1088: Road To Nano Technolgy education in engineering Technology : an area of interdisciplinary studies.
[3[E.N. Wikipedia. org / wiki/ carbon nanotubes.
[4] A seminar report / project – slide share (Nov. 26-2013)
[5] PhD thesis, theoretical study of electronic transport through bent carbon nano tube(2017) B.R.A.B.U. Muzafferpur, Bihar
[6] Physics of carbon nano tube by M.s.Dresslhaus and R.Saito, MIT(2008)
[7] J.A.Despres, E. Daguerre and K.Lafdi, carbon -33,87(1995)
[8] http://www.nanotech-now.com
[9] Electronic transport through bend carbon nanotube. Phys.Rev.B67, 205423(2003)
[10] A Rochefort, D.r.Salahub, and Ph.Avouris,Chem.Phys. Lett. 297,45(1998)
[11] A Rocherfort, Ph. Avouris,F. Lesage, and D.R.Salahub, Phys. Rev. B60,13824 (1999)
[12] T.W. Tombler. C.Zhou, L.Alexseyev, J. Kong, H. Dai, L. Liu, C. S. Jayanthi, C. Tang .and S. Y. Wu, Nature(London) 405, 769 (2000)
[13] M. Buttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B31,6207 (1985)