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Electrical Characteristics of Carbon Nanotubes

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Abstract: Carbon Nanotubes are the new wonder materials which have opened up new pathways in the field of electronics. CNTs due to their Chirality, they can act as metallic as well as semiconducting materials. In this review an attempt to study the electrical characteristics of Single Walled Carbon Nanotube has been made. A CNT molecule inserted between two gold electrodes and the variations in the electrical characteristics are observed by using Quantum wise Virtual Nanolab Software.

Keywords: Tunnelling; Transmission Coefficient; Transmission Spectrum; K-Point Sampling.

I. INTRODUCTION

The field of molecular electronics is particularly exciting because the possibility of engineering novel molecules that exhibit various kinds of I-V characteristics. Much work is done to measure the conductivity and other properties of individual molecules or to model electronic devices using them. There is evidence that molecules exhibit switching behaviour, although the precise mechanism is still unclear. The Non-Equilibrium Green's Function (NEGF) formalism that can be used in conjunction with a suitable molecular Hamiltonian (semi-empirical or ab initio) to investigate the I-V characteristics of different molecules.

Theoretical investigations can be used prior to experimentation to make approximations. The current-voltage characteristics thus obtained theoretically can be used to model the molecules as electron devices. So the current voltage characteristics have been obtained for the single walled CNT's [1].

In this paper the single walled CNT's are inserted between gold terminals to assemble two terminal structures. The software Virtual Nanolab is used to calculate the current flowing through the gold-Single walled CNT-gold assemblies for applied voltages. The molecules were explored extensively for there for their electrical properties by plotting current voltage characteristics. The curves of transmission spectrum and I-V characteristics display resonant tunnelling pattern. On the basis of the curves obtained the single walled CNTs are proposed as Resonant Tunnelling Diodes.

II. CURRENT VOLTAGE CHARACTERISTICS

An To study the current voltage characteristics the single walled CNT is placed between two gold electrodes one as source and other as drain. The gold-CNT-gold assembly is shown in following Fig.1.The voltage applied at the source fixing the drain potential is from -5 to 5V. This potential difference will maintain them at distinct potentials i.e.

$\mu_2 - \mu_1 = qVs$

giving rise to two different Fermi functions that

$f_1(E) = f_0(E-\mu_1) = \{1+\exp[(E-\mu_1)/K_BT]\}^{-1}$

$f_2(E) = f_0(E-\mu_2) = \{1+\exp[(E-\mu_2)/K_BT]\}^{-1}$

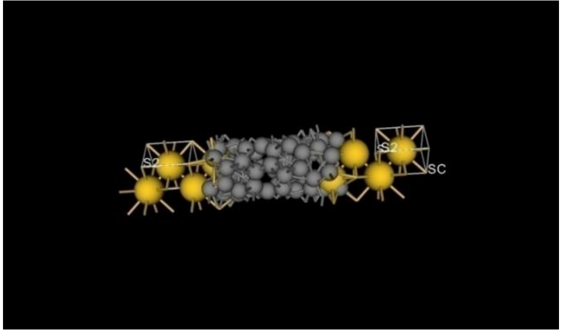

Fig 1 Gold-CNT-Gold Assembly

each contact seeks to bring the channel into equilibrium with itself. The quest to achieve equilibrium causes the current to flow from source to drain. The single walled CNT was inserted between two gold terminals in the two probe setup of virtual nanolab software with the contact arrangement showed in above figure. The molecules are chemisorbed onto electrodes, and the above orientation is fixed, although these molecules being asymmetric, the current voltage characteristics will be varying greatly with orientation [1,2]. A voltage bias varying from -5 to 5V was applied to CNTs of different radius and the corresponding current values are plotted.

III. TUNNELLING

A. Tunnelling through a Potential Barrier

In Nanoelectronic devices tunneling is a very important topic because it is used as variety of applications. To understand the concept of tunneling , let us consider an electron (a particle) incident from the left on a potential energy barrier. At that time potential energy profile is given by:

$$V = \begin{cases} Vo & , \ 0 \leq x \leq a \\ 0, & x < 0, x > a \end{cases}$$

Potential energy profiles an model an electron bound to a molecule, an electron bound to a quantum dot and similar confinement structures [3]. By assuming that the barrier does not contain any scattering objects , therefore the particles transfers the barrier coherently. Due to this assumption there is need to solve the Schrodinger's equation with boundary conditions applied at the barrier's interfaces but not at the various points inside the barrier.

Then two very interesting cases arise:
1) When the total energy E of the particle is greater than voltage Vo (E > Vo)
2) When the total energy E of the particle is less than voltage Vo (E < Vo)

In the first case when E > Vo the particle will simply move past the potential barrier with the 100 percent certainty. At that time its transmission coefficient would be unity and its reflection coefficient would be zero.
In the second case when E < Vo the particle would be reflected from the barrier with 100 percent certainty. At that time its transmission coefficient would be zero and its reflection coefficient would be unity.

B. Theory of Resonant Tunnelling through Molecules

The transport of electrons through molecules via the molecular orbitals. Adequate alignment of the Fermi energy of the metallic contacts with the molecular orbitals of the molecules results in creation of a channel for the flow of electrons from one terminal to other via the frontier molecule orbitals of molecular island. The required alignment can be achieved by applying bias on the metallic terminals called source and drain.

A molecule is characterized by the electrons occupying the molecular orbitals where each molecular orbital is identified by unique energy value. The molecular orbitals in which electrons reside are called occupied molecular orbitals and the empty one are called unoccupied molecular orbitals. The occupied molecular orbitals are separated from unoccupied molecular orbitals by an energy gap called HOMO-LUMO gap (HLG). When no bias is applied the Fermi level of the terminals lies in the middle of the HLG [5].

When positive voltage is applied on the source terminal, the terminal is depleted of electrons. So the Fermi level of source terminal is lowered while Fermi level of drain maintains its level in the middle of the HLG. Difference in potential induces flow of electrons through the HOMO of the molecule from drain to source. The current flows from source to drain depicting p-type of behavior by the molecule. As the value of voltage is further increased, more current flows through the probe setup. When the source is applied negative potential, it increases electron population resulting in elevation of the Fermi level of the source. When the energy of source is raised to the level of an unoccupied level, a channel is created for flow of electrons [4]. The electrons flow from source to drain resulting in current flow from drain to source, representing n-type of conduction. So it can be inferred that the electron flow will be blocked as long as the Fermi energy of the electron reservoirs (source or drain) lies somewhere in the HOMO-LUMO gap. The current flows through the molecule whenever the Fermi Energy of the reservoirs is duly aligned with the molecular orbitals whether the orbitals are occupied or unoccupied [6].

IV. TRANSMISSION COEFFICIENT

A transmission coefficient describes the amplitude intensity or total power of a transmitted wave relative to an incident wave. In quantum mechanics the transmission coefficient and reflection coefficient which is also related to it are used to describe the behavior of waves incident on a barrier. The transmission coefficient represents the probability flux of transmitted wave relative to that of the incident wave. It basically describes the probability of a particle tunneling through a barrier.

The transmission coefficient is defined in terms of the incident and transmitted probability current density J according to:

$$T = \frac{\vec{J}_{trans.} \cdot \hat{n}}{\vec{J}_{inc.} \cdot \hat{n}}$$

Where J_{inc} is probability current in the wave incident upon the barrier with normal unit vector $\hat{n}$ and J_{trans} is the probability current in the wave moving away from the barrier on the other side. The reflection coefficient R is defined as:

$$R = \frac{\vec{J}_{refl.} \cdot -\hat{n}}{\vec{J}_{inc.} \cdot \hat{n}} = \frac{/Jrefl/}{/Jinc/}$$

Conservation of probability implies that T+ R = 1, which is in one dimension reduces to the fact that the sum of the transmitted and reflected currents is equal in magnitude to the incident current.

V. TRANSMISSION SPECTRUM

The main quantity of interest in most calculations is transmission spectrum. The point at which the transmission is very high is known as the Fermi level. The transmission spectrum gives the comparison between the HUMO-LUMO gap of molecule and typical electron excitation energies. There are main two points which have to be noted in transmission spectrum graph these are:

1) If the highest peak or the peak of Fermi level is at point 1 in the graph of transmission spectrum then it shows the ohm's law.
2) If the highest peak is at point 2 in the graph then at that time the electron excitation energies are very high, due to this electrons crosses the barrier directly and shows the Resonant Tunneling.

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VI. K-POINT SAMPLING

The Au–CNT–Au interface system has periodic boundary conditions in the two directions parallel to the interface (the A and B directions). In these directions, the wave functions are Bloch waves and we must average over all the k-vectors when calculating physical quantities. In our two-probe calculation, two different quantities depend on the number of k-points used in the A and B directions. The first quantity is the the density matrix, the other is the transmission coefficient. Usually, it will require more k-points to accurately calculate the transmission coefficient, compared to the density matrix, and in VNL, it is therefore possible to specify different numbers of k-points for the two quantities. The number of k-points used for the density matrix is defined in the electrode input file. To understand why so many k-points are needed to converge the transmission coefficient, it is instructive to plot the k-dependence of the transmission coefficient. All the data used for calculating the k-point averaged transmission coefficient are stored in a net cdf data file.

VII. RESULTS AND ANALYSIS

A. Structure of Single Walled CNT with radius 1.988Å. The structure shown in Fig.2 is the 3 dimensional structure in which middle molecule is Carbon Nano tube (CNT) and there are two electrodes of gold one is left side and another is right side. There are two interfaces, one interfaces is between the left electrode and CNT and other interface is between the right electrode and CNT. There are two indices which defines the structure of CNT is chiral because the value of n = 6 and m = 2. The radius taken at that time is 1.988Å.

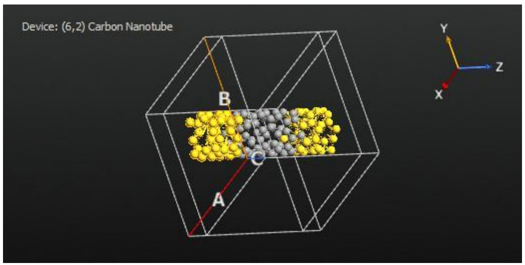

Fig.2 Structure of CNT with radius 1.988Å

The transmission spectrum and corresponding V-I Characteristics of CNT with radius 1.988Å are given in Fig. 3 and 4 respectively. There is electron excitation energy in one side and transmission energy on another side. $€_R$ and $€_L$ is the HUMO – LUMO gap in the transmission spectrum graph. According to the two cases which were discussed above in transmission spectrum the transmission is very high at 1.6(Fermi level) and at that point electron excitation energy is also very high.

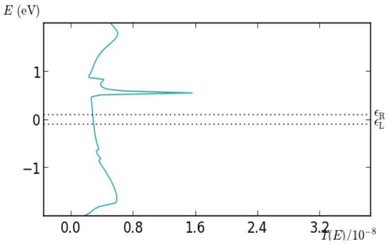

Fig. 3 Transmission spectrum of CNT with radius 1.988Å

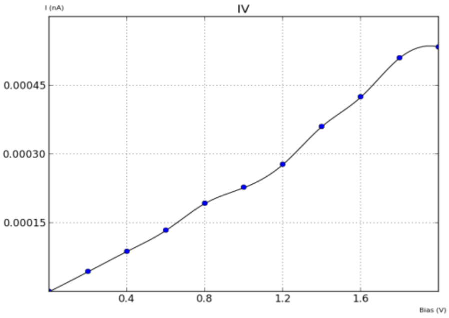

Fig. 4 V-I Characteristics of CNT with radius 1.988Å

As in the transmission spectrum the highest peak is very close to 1, therefore the graph is almost linear thus following ohm's law. The conductivity of CNT with radius 1.988Å is very high at that point. The graph is almost linear therefore it act as a resistor. Moreover the conductivity of CNT is very high at that time.

B. Structure of Single Walled CNT with radius 2.66Å

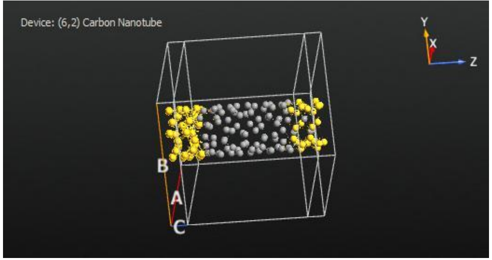

Fig. 5 Structure of CNT with radius 2.66Å

The Fig.5 shows structure of CNT of radius 2.66Å. The value of indices of this CNT is n= 6 and m = 2 which shows the chiral structure of the CNT. The chiral structure of CNT always shows semiconducting nature. The corresponding transmission spectrum and V-I characteristics od CNT is is given in Fig. 6 and 7. In this graph of transmission spectrum, the transmission energy is very high just above 2. Therefore that point shows the Fermi level of electrons

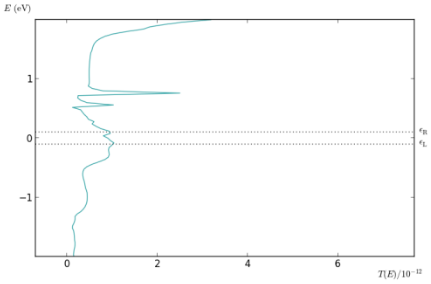

Fig. 6 Transmission spectrum of CNT with radius 2.66Å

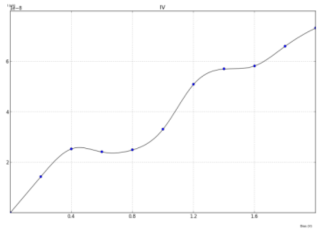

Fig. 7 V-I characteristics of CNT with radius 2.66Å

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The V-I curve shows tunnelling at point 0.4 and upto 0.4 point the value of resistance is 0.153 x 10^9 Ω. After that there is small amount of voltage drop from 0.4 to 0.8. Voltage drop from 0.4 to 0.8 shows the negative resistance of -2 x 10^9Ω. Then again tunnelling is shown from 1.2 to 1.6 and up to that point the value of resistance is 2 x 10^9Ω. From this we can conclude that a sudden increase in resistivity occurs from negative to positive value of resistance. Therefore overall conductivity is decreased of CNT of radius 2.66Å than the CNT of radius 1.988 Å.

C. Structure of Single Walled CNT with radius 3.081Å

The single walled CNT with radius 3.081Å is shown below in Fig.8. As compare to the CNT with radius 2.66Å in this case the radius is increased upto 3.081Å. The change in the transmission spectrum and V-I curve are discussed below.

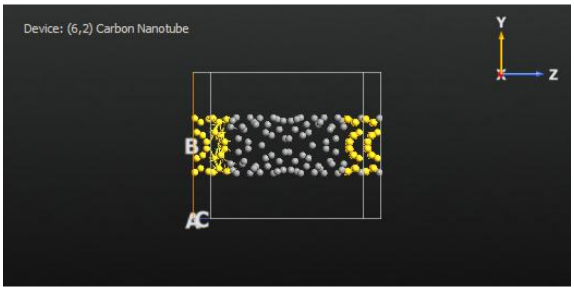

Fig. 8 Structure of CNT with radius 3.081Å

The transmission spectrum and V-I characteristics of CNT are shown below:

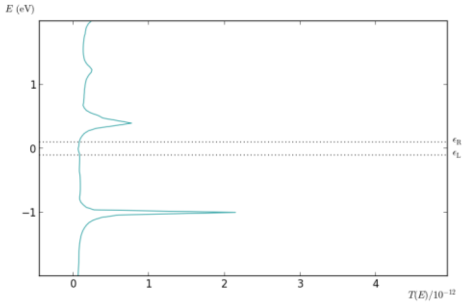

Fig.9 Transmission Spectrum of CNT with radius 3.081Å

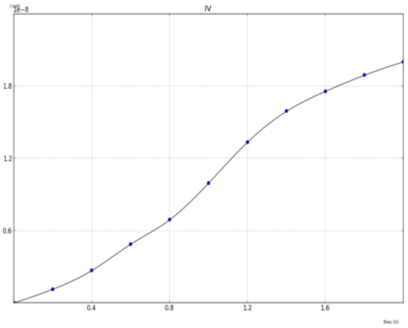

Fig.10 V-I Characteristics of CNT with radius 3.081Å

In the graph of transmission spectrum the highest peak of transmission energy is above the 2 and at that point electron excitation energy is also very high. The electron excitation energy is at -1 therefore the conductivity of the CNT is negligible in this case.

If we see in Fig.10 it is almost straight line but from the value of resistance i.e. 1 x 10^9 Ω the resistivity is very high and due to this the value of current is very low. Therefore we can say that by increasing the radius of single walled CNT from 2.66Å to 3.081Å the conductivity is decreased. In the following graph there is slightly tunneling is shown from 0.8 to 1.6.

D. Structure of Single Walled CNT with radius 4.976Å

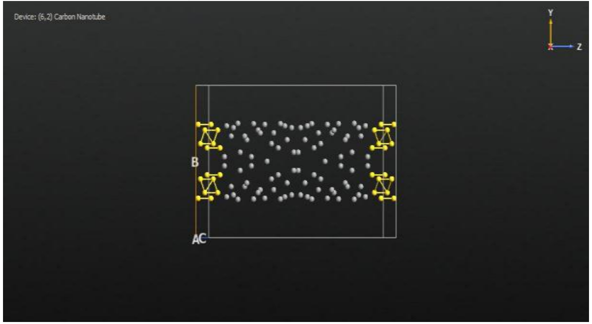

Fig. 11 Structure of CNT with radius 4.976Å

The Fig.11 shows the 3 dimensional structure of CNT with 4.976Å radius There are two interfaces, one interfaces is between the left electrode and CNT and other interface is between the right electrode and CNT. There are two indices which defines the structure of CNT is chiral because the value of n = 6 and m =2. The radius taken at that time is 4.976Å. The corresponding Transmission spectrum and V-I characteristics are shown below in Fig. 12 and 13 respectively.

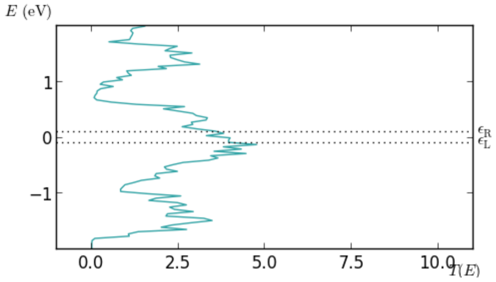

Fig.12 Transmission spectrum of CNT with radius 4.976Å

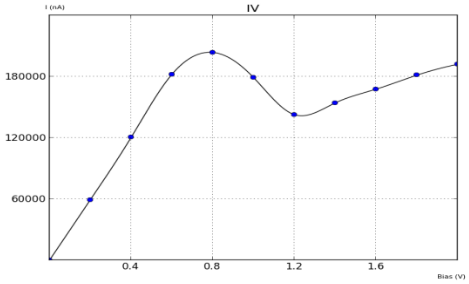

Fig. 13 V-I Characteristics of CNT with radius 4.976Å

In the graph of transmission spectrum, the transmission energy is very high at 5.0. Therefore 5.0 point shows the Fermi level of excitation of electrons. The V-I curve of the CNT shows tunneling at 0.8 point and upto 0.8 point CNT follows the Ohm's Law and the resistance upto this point is 0.034 x 10^5 Ω. Then there is sudden voltage drop from 0.8 to 1.2 or also shows tunneling from 0.8 to 1.2

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and at that point the value of resistance is -0.04 x $10^5\Omega$. Then after 1.2 point the bulk device again follow the Ohm's Law and after 1.2 point the value of resistance also changed from negative resistance to positive resistance i.e. 0.133 x $10^5\Omega$. The overall conductivity is decreased with increasing the radius of CNT.

E. Structure of Single Walled CNT with radius 5.367Å

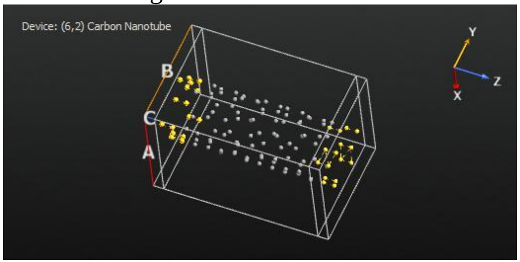

Fig.14 Structure of CNT with radius 5.367Å

The Fig. 14 shows the structure of CNT with radius 5.367Å. There are two indices which defines the structure of CNT is chiral because the value of n = 6 and m = 2. If n > m then the structure is chiral, when n= m then the structure is armchair and when n = some value and m = 0 then the structure will be zigzag. The corresponding transmission spectrum and V-I Characteristics of CNT are given below in Fig.15 and 16 respectively.

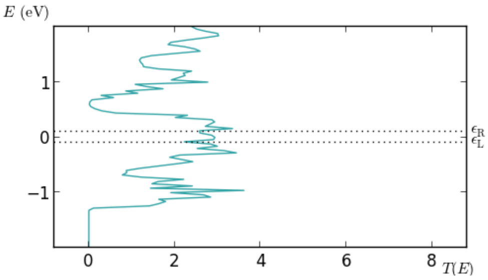

Fig. 15 Transmission spectrum of CNT with radius 5.367Å

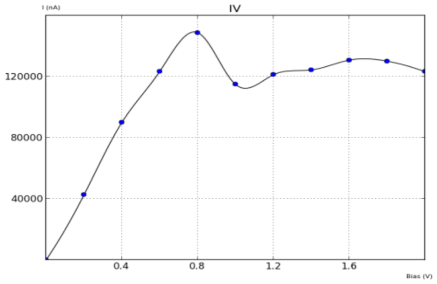

Fig. 16 V-I Characteristics of CNT with radius 5.367Å

In the graph of transmission spectrum the highest peak of transmission energy is near the point 5 and at that point electron excitation energy is also very high. The electron excitation energy is at -1. Due to these electrons crosses the barrier directly and shows the Resonant Tunneling. But in this case the highest peak is at point -1 therefore the conductivity of CNT is negligible in this case. In the V-I Graph upto point 0.8 the value of resistance is 0.053 x $10^5\Omega$ and also the resistance during tunneling from 0.8 to 1.2 is -0.0057 in micro ohm ($\mu\Omega$). After that from point 1.2 to 1.6 the value of resistance is 0.4 x $10^4\Omega$. Then between 1.6 and 2.0 voltage bias again negative resistance is observed. From this graph we can conclude that if the radius of single walled CNT is increased from 3.081Å to 5.367Å then in the V-I graph there will be tunneling at various points. Due to this there is various ups and downs in the conductivity of the CNT. Therefore overall conductivity of CNT is decreased.

VIII. COMPARISON OF ALL RESULTS

On the basis of two conditions of transmission spectrum all results which are showing below are discussed i.e.

1) If the highest peak or the peak of Fermi level is at point 1 in the graph of transmission spectrum then it shows the ohm's law.
2) If the highest peak is at point 2 in the graph then at that time the electron excitation energies are very high, due to these electrons crosses the barrier directly and shows the Resonant Tunneling.

TABLE I: CONDUCTIVITY CORRESPONDING TO VARIOUS PEAKS OF TRANSMISSIONS SPECTRUM

Radius of CNT	**Highest Peak in Transmission Spectrum**	**Conductivity**
1.988Å **2.66Å** **3.081Å**	**Almost 1** **Almost 1** **-1**	**Ohm's Law** **Ohm's Law** **Tunnelling Diode**

As we can see in the table 4.2 the highest peak of transmission spectrum is decreased from 1 to -1 as we in the radius of the CNT. Moreover the conductivity of the single walled CNT is decreased by increasing the radius. In this chapter the preliminary investigations of the current voltage characteristics of single walled CNTs of different radius have been carried out. The curves are marked by presence of peaks in the negative resistance section. These peaks imply resonant tunnelling that is displayed whenever Fermi level is aligned to an occupied or unoccupied molecular orbital.

TABLE II: VARIATIONS IN THE ELECTRICAL CHARACTERISTICS WITH RADIUS

Radius of CNT	**CNT Functions**
1.988Å	Resistor
2.66Å	Resistor
3.081Å	Resistor
4.976Å	Tunneling Diode
5.367Å	Tunneling Diode

If we see in the Table II one side there is radius of CNTs starting from 1.988Å to 5.367Å and the other side shows the functions of CNT. As the radius of CNT is increased from 1.988Å to 5.367Å the corresponding change in functions of CNTs were observe.

Upto radius 3.081Å the CNT was act as resistor and follow Ohm's Law. But when the radius is increased then

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CNT shows tunneling and act like a tunneling diode as shown in the table 4.4. Therefore from the observations the CNTs shows tunneling effect as we increase the radius. Now there are some changes in the C-C bond length and the length of CNT of various samples taken. These all variations are shown below.

TABLE IV: BONDLENGTH AND CORRESPONDING LENGTH OF CNT SAMPLES

Radius of CNT (Å)	C-C Bondlength (Å)	Length of CNT(Å)
1.988	1	10
2.66	1.34	14
3.081	1.55	16
4.976	2.5	27
5.367	2.7	29

The Table IV shows the C-C bond length and length of various samples of CNT which were taken in this thesis. As the radius of CNT is increased the corresponding bond length and length of CNT is also increased. In the table we can see that as the radius is increased from 1.988Å to 5.367Å and the corresponding bond length is increased from 1Å to 2.7Å. Also the length of CNT is also increased from 10Å to 29Å.

IX. CONCLUSION

In this paper we conclude that there are various changes are observed in electrical conductivity of the CNTs with change in radius of CNTs. CNTs with small diameters are more conductive then the CNTs with large diameters. Moreover as we increase the radius of CNT it shows the tunneling effect. This is due to unique energy levels of the molecular orbitals. Although the magnitude of current that flow through these devices reduces but the current density is extremely large. CNT has already captured its importance in Nano electronics because of its unique properties like high electrical conductivity and high tensile strength.

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BIOGRAPHIES

Ruhee, pursuing M.Tech in the field of Electronics and Communication. Her thesis is the study of the variation in the electrical conductivity of carbon nano tubes. Her publications include review papers on Carbon Nanotubes published in a National Conference, Review on Fullerenes, published in an International Conference. Review on Nanoelectronics, published in the International journal IJARSE and poster published by International Nano Science Community.

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