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Theoretical Approach of Conductance of Armchair Carbon Nanotubes

Hemendra Kumar
Assistant Professor,
Dept. of Physics,
MMH College,
Ghaziabad, U.P., India

Sanjeet Pratap Singh
Assistant Professor,
Dept. of Physics,
MMH College,
Ghaziabad, U.P., India

Abstract

In the present work, authors have calculated the conductance of armchair carbon nanotubes. Before the computing of conductance, carriers current is calculated by Landaur-Buttiker formula. For the calculation of electron density in carbon nanotubes we have used the Thomas-Fermi approximation method. It serves to estimate the charge density without invoking a solution of the Schroedinger equation for all energy levels.

Keywords: Landaur-buttiker, CNT

Introduction

Nanotubes were discovered quite accidently by Sumio Iijima [1] while studying the surfaces of graphite electrodes used in an electric arc discharge. Carbon nanotubes having good electrical properties cause of this features carbon nanotubes use as emitter devices. When small electric field is applied to the axis of the nanotube, electrons are emitted at very high rate from the ends of the tube. This phenomenon is called field emission. In other words we can say that emission of electron from parent atom in the presence of the high electric field is known as field emission. High thermal and electrical conductivity of carbon nanotubes make them as one of the important field emitters. One reason for the high conductivity of the carbon tubes is that they have very few defects to scatter electrons, and thus a very low resistance. Magneto resistance is a phenomenon whereby the resistance of a material is changed by the application of a DC magnetic field. Carbon nanotubes display magneto resistive effects at low temperature. It is seen that, this is a negative magneto resistance effect because the resistance decreases with increasing DC magnetic field, so its reciprocal, the conductance G=1/R, increases. This occurs because when a DC magnetic field is applied to the nanotubes, the conduction electrons acquire new energy levels associated with their spiraling motion about the field. It turns out that for nanotubes these levels, called Landau levels, lie very close to the topmost filled energy levels (the Fermi level). Thus there are more available states for the electrons to increase their energy, and the material is more conducting. The electrically conductive material can be made with help of carbon nanotubes [2]. In this work we use the Thomas – Fermi approximation to considering the electron density. With the help of electron density we calculate current at different voltage then conductance easily calculated.

Objective of the study

When a large number of CNTs is placed perpendicular to the electrodes, electron emission can be observed. This technique is being used in flat panel displays. Television and computer monitors contain a controlled electron gun to impinge electrons on the phosphorus of the screen, which then emit light of the appropriate colors. Carbon nanotubes have been regarded as a promising field electron emission source for the field emission displays [FEDs] and vacuum electronic devices [3]. Field electron emission involves a quantum mechanical tunneling process under an applied electric field. CNTs are used as field emitters having field emission parameters such as Turn-on-field, current density, mean field enhancement factor by Park [4], and others as conductance. So conductance is a parameter which can varies the features of CNT such as conductivity. CNTs have good conductance properties are use in field emission devices.

Review of Literature

The role of Conductance is most important in carbon nanotubes to measuring the conductivity. Many researchers worked on electrical conductivity of CNT. Conductance play a important role to measuring the thermal conductivity of CNT in different model. The general model for calculating the tube-tube contact conductance of a single thermal contact is given by X.Yang. A theoretical prediction models for the thermal conductivity of a random CNT network is given by various researchers,the model for a partially welded random network proposed by the Yang X.M.[5]. These models have been used in the thermal conductivity analysis by Zhang K.J.[6].

Concepts

In this work we have calculated the electron density of carbon nanotubes with respect to their diameter. For the calculation of electron density in carbon nanotubes we have used the Thomas-Fermi approximation method. It serves to estimate the charge density without invoking a solution of the Schroedinger equation for all energy levels. This approximation method takes the response of the electron gas to an externally applied potential. The electron density is computed by Thomas – Fermi approximation and given by [7]

$$n(x,T) = \int_0^{\infty} g(E)\left[1+\exp\left\{\frac{E-E_F-eV_{ext}}{k_BT}\right\}\right]dE \qquad (1)$$

Where $g(E)$ is the density of states in the semiconductor. The preceding equation is then evaluated as

$$n(x,T) = N_e(x,T)F_{\frac{1}{2}}\left\{\frac{E_F+eV_{ext}}{k_BT}\right\} \qquad (2)$$

Where, $N_e = 2\left[\frac{m_e k_B T}{2\pi\hbar^2}\right]^{\frac{3}{2}}$ and m_e is the effective mass of electron and $F_{\frac{1}{2}}$ is the Fermi-Dirac integral conventionally defined by

$$F_\alpha(\eta) = \frac{1}{\Gamma(\alpha+1)}\int_0^{\infty} E^{\alpha}\left[1+\exp(E-\eta)\right]^{-1}dE \qquad (3)$$

After solving these equations the electron density per unit length of CNT is given by Thomas-Fermi approximation and calculated value for different diameter of CNT is given by equation

$$N_e = 15.065\times10^{24}(d_{CNT})^2 e^{\left(\frac{E_F+eV}{k_BT}\right)} \qquad (4)$$

We have calculated the conductance of carbon nanotube field effect transistors, which is denoted by G =dI/dV.

Research Design

Before the computing of conductance carriers current is calculated by Landaur-Buttiker formula [8].

$$I = \frac{4q}{h}\int f(E).TC(E).dE \qquad (5)$$

In equation (5), TC(E) is the transmission coefficient of electrons, its value is taken unity in this work and f(E) is the Fermi statistic. So equation (5) is rewritten in the form

$$I = \frac{4q}{h}\int \frac{1}{1+e^{\left(\frac{E-E_F}{k_BT}\right)}}dE \qquad (6)$$

In equation (6) *h* is the Planck constant and *q* is the total charge in the system. N_e is the total number of electrons per unit length of CNT. Thus the total charge *q* in CNT will be

$$q = N_e \times e \qquad (7)$$

Where *e* is the charge of electron. With the help of equations (5), (6) and (7) the carrier current is given by

$$I = -\frac{60.260\times10^{24}\times e}{h}(d_{CNT})^2 e^{\left(\frac{E_F+eV}{k_BT}\right)}\times k_BT\times \log[1+e^{-\left(\frac{E-E_F}{k_BT}\right)}] \qquad (8)$$

Thus the conductance is given by

$$G = \frac{dI}{dV} \qquad (9)$$

We have computed the conductance with the help of equation (8) and (9) which is given by

$$G = -23.374\times10^{20}(d_{CNT})^2 e^{\left(\frac{E_F+eV}{k_BT}\right)}\times \log[1+e^{-\left(\frac{E-E_F}{k_BT}\right)}] \qquad (10)$$

In equation (10), *E* is the angular energy level of CNT, in this work we have taken the value of *E* is E_0 with respect to different diameter of CNT, which is calculated by equation

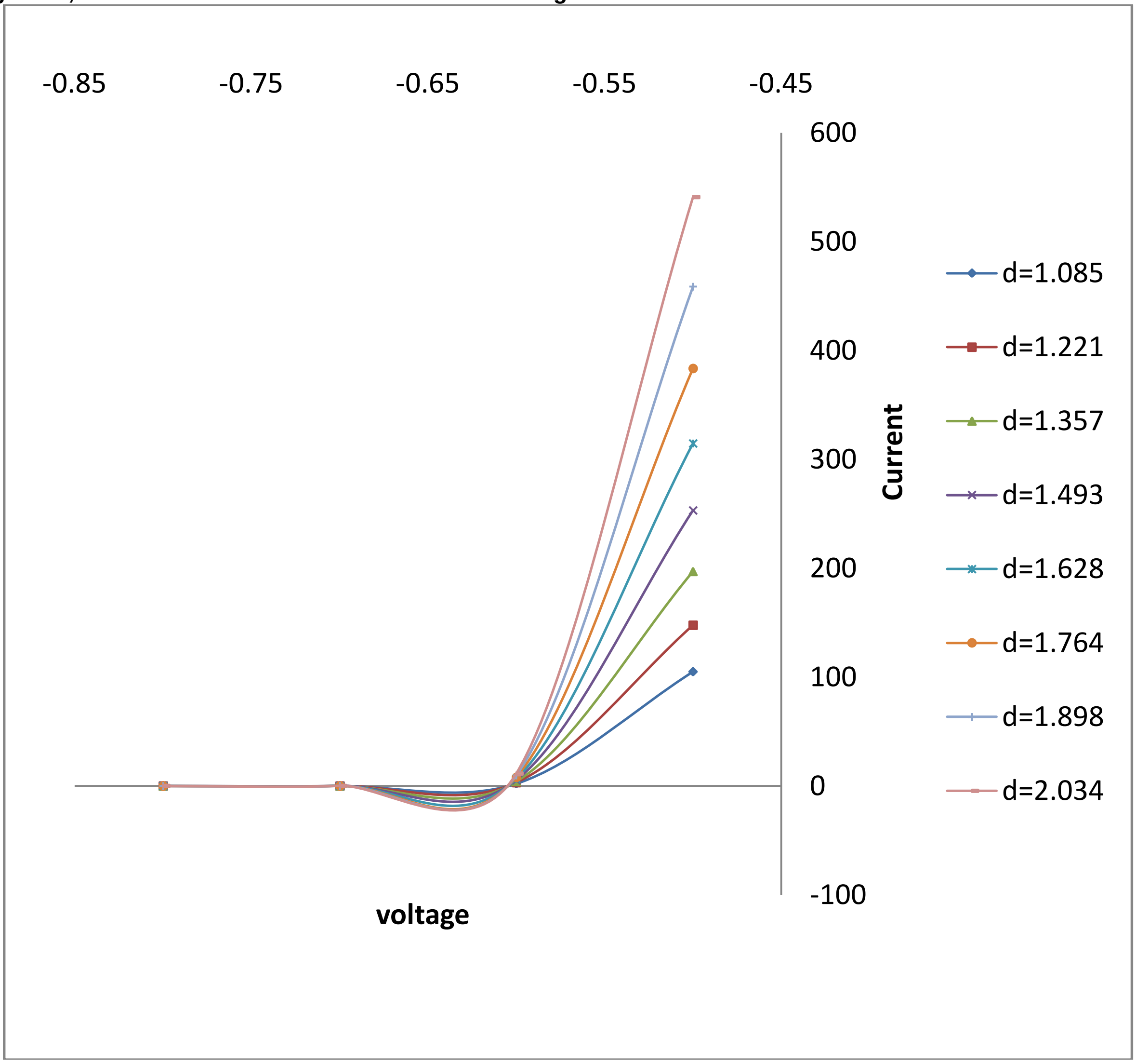
$$E_m = \frac{|3m+1||V_{PP}|a_{cc}}{d_{CNT}}$$

E_F is the Fermi energy level and its value is 0.625eV taken in this work. V is the applied external voltage and k_B is the Boltzman constant and all calculations are made at room temperature i.e. T=300K, d_{CNT} is the diameter of the carbon nanotubes. With the help of equation (8) we have described the behavior of the I-V characteristic of carbon nanotubes, in this equation (8) negative sign gives the direction of current. The calculated values of current as a function of diameter for armchair carbon nanotubes are given in Table 1 .A graphical representation current versus voltage is shown in

Table 1; Current as a Function Of Voltage For Different Diameter of Armchair Carbon Nanotube

S.No.	Voltage in Volts	Current in k Ampere For Different Diameter							
		1.085	1.221	1.357	1.493	1.628	1.764	1.898	2.034
1	-0.5	104.950	147.780	197.223	253.327	314.794	383.780	458.655	540.894
2	-0.6	2.240	3.157	4.210	5.412	6.725	8.199	9.790	11.556
3	-0.7	.048	.067	.090	.116	.144	.175	.209	.247
4	-0.8	.001	.001	.002	.002	.003	.004	.005	.005

Figure 1 ; Variation of Current As A Function of Voltage for Various Diameter of Armchair Carbon Nanotube

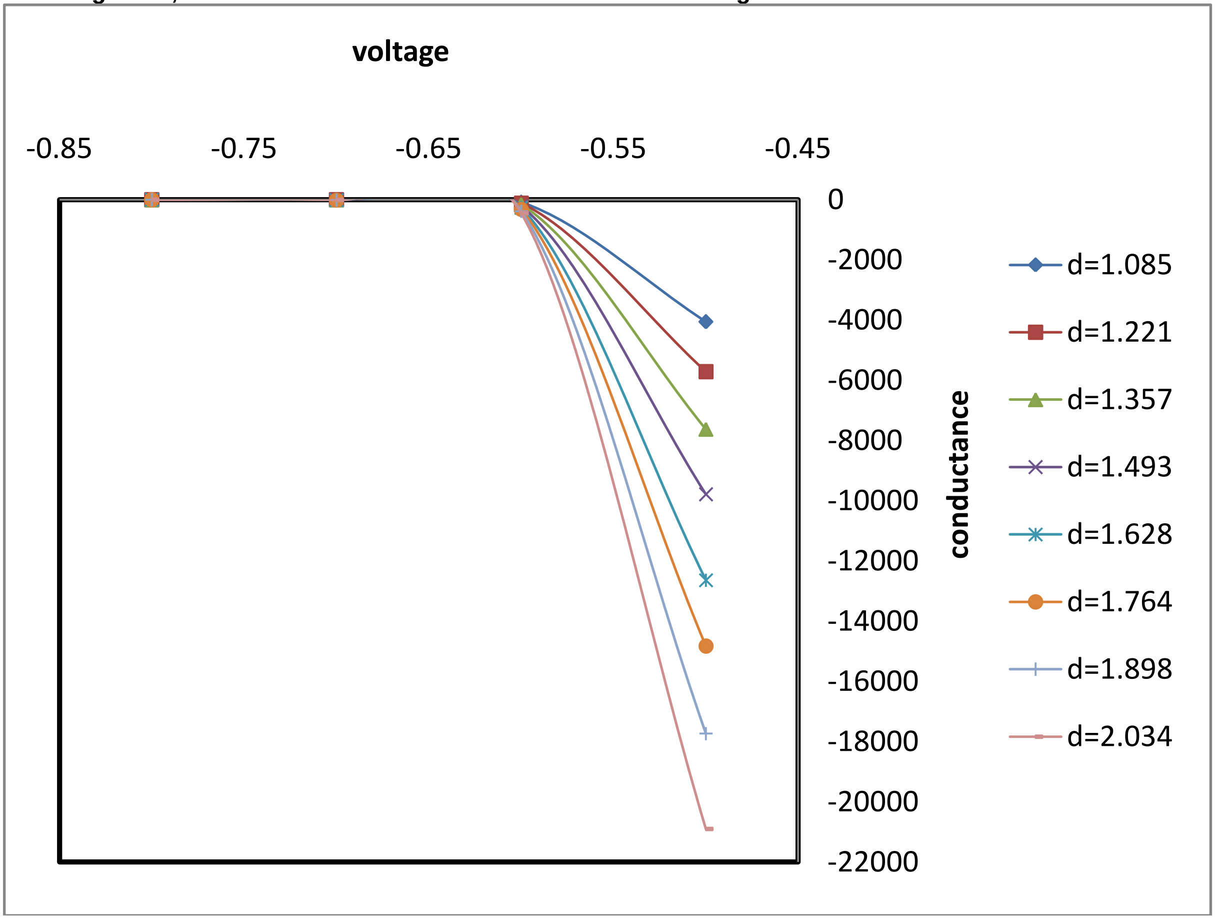


The calculated conductance dI/dV at different voltages for armchair carbon nanotubes for different diameters is given in Table 2. A graphical representation of dI/dV as a function of voltage is shown in Figures 2.

Table 2 ; Conductance as a function of voltage for different diameter of armchair carbon nanotube.

S.No.	Voltage in Volts	Conductance of carbon nanotubes in $K\Omega^{-1}$ for different diameter							
		1.085	1.221	1.357	1.493	1.628	1.764	1.898	2.034
1	-0.5	4056.037	5711.340	7622.132	9790.459	12633.272	14832.149	17725.852	20904.187
2	-0.6	86.653	122.017	162.839	209.163	269.897	316.874	378.695	446.597
3	-0.7	1.851	2.606	3.478	4.468	5.765	6.769	8.089	9.540
4	-0.8	0.040	0.056	0.074	0.095	0.123	0.145	0.173	0.204

Figure 2 ; Variation of Conductance as A Function of Voltage For Armchair Carbon Nanotubes



Conclusion

From Figures 1 it is clear that when negative voltage increased there is no more current found upto -0.6V but voltage reduces below -0.6V exponentially current increased. Thus we can say this gives good agreement of current at low voltage. In other words we conclude that upto a certain voltage the I-V characteristics are non-Ohmic which would indicated that a barrier potential exists somewhere along this conduction path, possibly due to high contact resistance at electrodes at carbon nanotubes. Furthermore, for a certain applied voltage current exponentially increased. A graphical representation of current for different diameter of carbon nanotubes are also shown in Figure 1. From Figures 2 it is clear that when applied negative voltage varies the conductance also varies. In other words we can say that when applied negative voltage increase the conductance dI/dV decreases. But due to negative sign we conclude that conductance is directly proportional to the applied negative voltage. The conductance of the carbon nanotubes varies from $k\Omega^{-1}$ to $M\Omega^{-1}$.

Endnotes

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