ISSN: 2319-8753

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 3, Issue 11, November 2014

Investigation of Doping Effects on Electronic Properties of Two Probe Carbon Nanotube System: A Computational Comparative Study

Khurshed A. Shah[1], Jehangir Rashid Dar[2]

Head of Department, Department of Physics, Govt. Degree College for Women, Anantnag, J&K, India[1]

Project Fellow, Department of Physics, Govt. Degree College for Women, Anantnag, J&K, India[2]

ABSTRACT: This paper reports the effect of various dopants on the electronic properties of Zig-Zag (4, 0) semi-conducting single walled two probe Carbon Nanotube system using first principle calculations and Non-Equilibrium Green's Function (NEGF) method. The modeled Zig-Zag (4,0) single walled Carbon Nanotube was doped with atoms of elements Tellurium (Te), Antimony (Sb), Arsenic (As) & Chromium (Cr) using Atomistic Tool Kit (version 13.8.1) software and its graphical interface (custom analyzer) Virtual Nanolab. The simulations were carried out in device mode using Density Function Theory (DFT) calculations. The current-voltage (I-V) characteristics & conductance of the four proposed models were studied for comparative study under low-bias conditions. The results show that Arsenic doping has increased the conductance of the model manifold than other doping atoms whereas Chromium doping has showed an amazing property of Negative Differential Resistance (NDR). Hence, we conclude that the proposed model is suitable for use in various CNT based high speed nanoelectronics applications including amplification, oscillation and arithmetic architectures.

KEYWORDS: Carbon Nanotube device, Non-Equilibrium Green's Function, Doping, Density Function Theory, ATK.

I.INTRODUCTION

Carbon Nanotubes have drawn great attention in both academic and industrial circles due to their wide potential applications. Since their discovery in 1991 by Sumio Iijima [1], carbon nanotubes have been subject for intense scientific and engineering research. It is because of its unique and remarkable mechanical, electronic, optical and chemical properties that this material has wide range applications in nanoelectronics, sports gear, lightweight super strong materials, renewable energy developments, tissue engineering and also in medicine [2-6]. In recent years, carbon Nanotubes based nanoelectronics has received much attention because of its tremendous potential in various applications such as active components, switches, memory devices, display devices and sensors [7]. Nanotubes are of two type's single walled and multi-walled nanotubes having chiral, Zig-Zag and armchair geometries. The nanotubes can be metallic or semiconducting depending on their chilarity and in a bundle sample one third of CNTs are metallic in nature [8]. Furthermore, carbon nanotubes can serve as an excellent media to address some quantum phenomena related to size effects such as ballistic transport, super current and universal conductance fluctuations [9]. It is necessary to further address whether the transport of carbon nanotubes is controlled by ballistic or diffusive mechanism and how the doping effects the electrical properties of carbon nanotube which is very important in the bandgap design engineering [10].

Since 1968 energy band engineering technique such as doping has played an important role in electronic industry in order to increase conductivity of silicon or germanium materials [11]. In the past decade lot of interest has been shown in doping the carbon nanotubes by different techniques to find out unexposed characteristics of carbon nanotubes [12-13].The electronic properties of carbon nanotubes can be deliberately modified. By proper choice of type of modification the electronic properties of carbon nanotubes can be tuned to a great extent. One of the methods of tuning electronic properties of carbon nanotubes is doping. The unique morphology of nanotubes mean there are a wide variety of possible approaches to dope carbon nanotubes thereby change their physical and electronic properties. Many of these take advantage of the molecular nature of the nanotubes, however it is also possible to dope in the more

DOI: 10.15680/IJIRSET.2014.0311044

ISSN: 2319-8753

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Vol. 3, Issue 11, November 2014

traditional sense i.e. deliberately replacing carbon nanotubes with impurities. To the best of our knowledge Boron and Nitrogen doping of carbon nanotubes has been done extensively by researchers [14], however no effort has been made to dope the CNTs by other elements including Tellurium (Te), Antimony (Sb), Arsenic (As) and Chromium (Cr). Therefore, to exploit CNTs in electronic industry it is important to investigate the doping influence of these elements on the electronic properties of two probe CNT system and this work is an initiative in that direction. It is pertinent to mention that several groups have used the doped carbon nanotubes in CNT field effect transistors, CNT complementary field effect transistors and in logic gates [15-17].

In this paper, we have adopted conventional method of doping for investigating the effect of dopants on the electronic transport properties of single walled carbon nanotube two probe system by applying Non-Equilibrium Greens Function (NEGF) formalism in combination with the first principle theory. The current-voltage characteristics of the device were visualized in order to analyze and investigate the best model for conductivity enhancement. The distinct change in conductance is reported as the type of dopant is varied in the central region of the carbon nananotube between the two on tube electrodes under low-bias conditions. From the results, it is clear that the Arsenic shows enhanced conductivity whereas Chromium doping has shown NDR which will find enormous applications in electronic industry.

The study is organized as follows. In section II, a brief overview about materials and methods used in modeling of the device is presented. In section III, a complete theoretical background of model with special emphasis on Landauer-Buttiker formalism is presented. Simulation results are presented in section IV. Section V concludes the paper.

II. MATERIALS AND METHODS

We modeled a Zig-Zag (4,0) single walled carbon nanotube using ATK (13.8.1) software and doped the scattering region with atoms of four different elements and then configured the set up for device mode as shown in the Figure 1(a, b) in order to find out the best dopant interms of current carrying capabilities for various electronic applications.

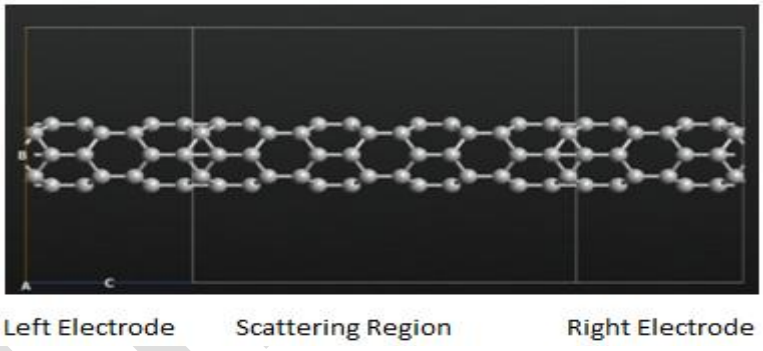

Figure 1(a): Model of pure two probe CNT system using Zig-Zag (4, 0) CNT.

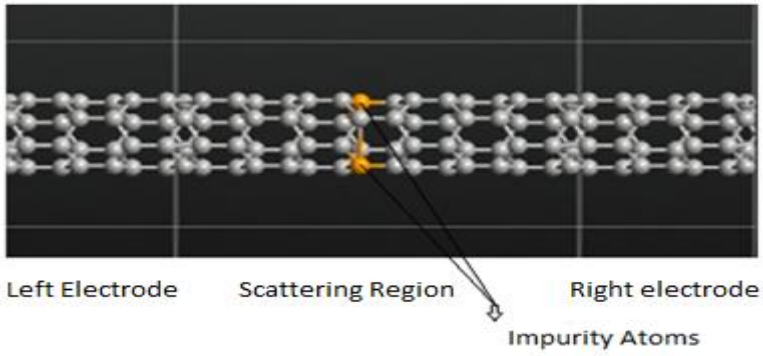

Figure 1(b): Model of 2 atom doped two probe CNT system using Zig-Zag (4, 0) CNT.

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The on tube device consists of three parts i.e, left electrode, scattering region and right electrode as shown in Figure 1(a). The scattering region is doped with dopant atoms of four different elements and as a model is depicted in Figure 1(b). The carbon-carbon bond length was selected as 1.42086 A° and length of two electrodes was considered to be 7.1043A° for better geometry optimization. 10% of the length of electrodes (0.7104 A°) was considered as scattering region in order to compensate for scattering losses at the joining ends of the central molecule and the left-right electrodes. Thus we modeled a two probe system consisting of a doped carbon nanotube inserted between two electrodes to predict the electronic transport through the junction under low bias conditions. Here we assumed that under the simulated conditions, inelastic scattering processes are negligible and thus we are dealing with an effectively ballistic transport. The hypothesis for this electron transport was based on Non Equilibrium Green's Function (NEGF) formalism [18]. We adopted the single particle approach to transport modeling, which is based on Landauer-Buttiker formalism. The selected DFT simulation parameters of the calculations are as follows:

1) Electron Temperature = 300K.
2) Density mesh cut-off = 75 Hartee.
3) K-point sampling = (1, 1,100).
4) Exchange Correlation = Local Density approximation (LDA) with single zeta polarized basis set.

These parameters were taken for calculations to be optimal combination of accuracy and speed. We adopted Fast Fourier2D solver as a Tool for Poisson solver of the boundary conditions and varied the applied bias across the two electrodes in the range of 0-1 Volt and measured the effective variation in the values of current and conductance.

III. THEORETICAL BACKGROUND

Density Function Theory (DFT) is presently the most successful and also the most promising approach to compute the electronic structure of matter. Walter Kohnn was awarded with Noble Prize in 1998 for the development of the Density Function Theory [19]. Its applicability ranges from atoms, molecules and solids to nuclei and quantum and classical fluids. In its original formulation, Density Function Theory provides the ground state properties of a system, and electron density plays a key role. Density Function Theory has been worked upon by various researchers for calculating the electron transport through single molecule junction [20]. The computation has been based upon Hartee-Fock method approximation for determination of ground state wave function given by

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\left(\frac{m\omega}{\hbar}\right)x^2}$$

where h= Planck's constant, ω = angular velocity and ground state energy $E_o = 1/2\hbar\omega$ of a quantum many body system along with Keldysh's Non-Equillibrum Green's Function (NEGF) formalism combined. The off diagonal matrix elements are calculated using Wolfsberg and Helmoltz approximation that relates them to the diagonal element and overlap matrix element.

According to the transport theory in low dimensional systems, the quantum step behavior in transport of carbon nanotubes was attributed to the two conducting transverse modes ($2G_o$) where $G_o=2e^2/h$ [21-23], where e the charge of an electron= $1.6\text{x}10^{-19}$ C and h Planck's constant. In these reports current was calculated by Landaur-Buttiker formalism, which give rise to the conductance of low-dimensional systems i.e, nanobased electronic devices interms of the electron transmission coefficient from left to right electrode. The Landauer-Buttiker (LB) method establishes the fundamental relation between the wave functions (scattering amplitudes) of an non-interacting quantum systems and its conducting properties. Therefore the Landauer-Buttiker method can be applied to find the current through a non-interacting quantum system or through an effectively non–interacting quantum system. According to Landaur, the current through the junction occurs due to the elastic scattering between two electrodes. The current calculated by Landaur-Buttiker [24-25] formalism is given by

$$I(V_b) = \frac{2e^2}{\hbar}\int_{u_L}^{u_R} T(E,V,b)dE$$

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Where $2e^2/\hbar$ is the quantum unit of conductance, T(E,V,b) is the transverse function, $\mu_L(V_b) = \mu_L(0) + eV_b/2$ and $\mu_R(V_b) = \mu_R(0) + eV_b/2$ are the chemical potentials of left /right electrodes, with $\mu_{L/R}(0)$ being the average Fermi level of the system and bias voltage is represented by $V_b = (\mu_L - \mu_R)/e$.

IV. SIMULATION RESULTS

In order to understand the effect of dopants on the conductance of Zig-Zag (4,0) single walled carbon nanotubes, the four proposed models were simulated in device mode using Atomistic Tool Kit (13.8.1) and its graphical interface (custom analyser) Virtual Nanolab [26]. The simulations were performed at different bias voltages in the range 0-1V. The Transmission Spectrum for all simulated models were analyzed by plotting I-V and conductance curves with respect to different applied bias voltages. Figure 2(a,b,c,d) shows I-V and dI/dV curves of four proposed models doped with 2 atom of Tellurium (Te), Antimony (Sb), Arsenic (As) & Chromium (Cr) respectively.

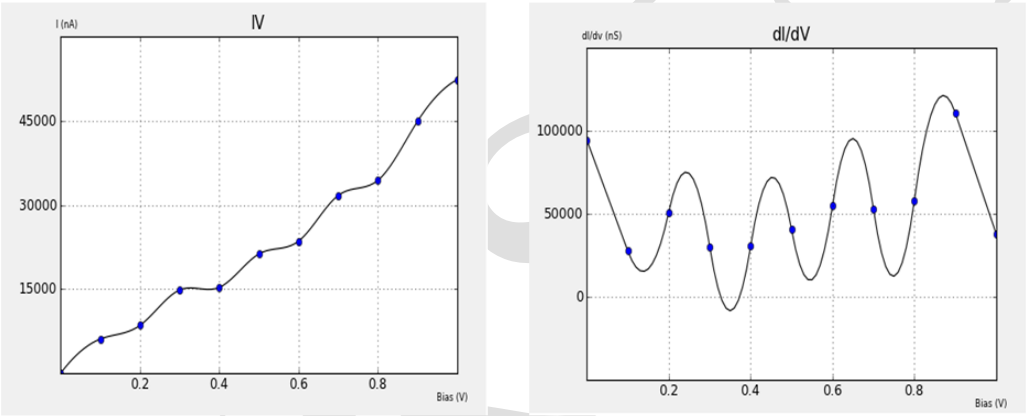

Figure 2(a): I-V& dI/dV curves for Tellurium (Te) doped two probe CNT system

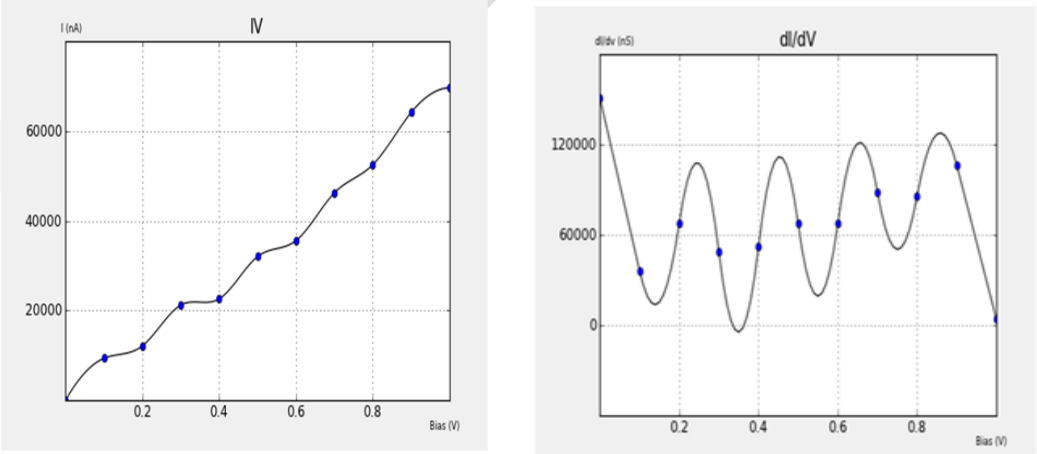

Figure 2(b): I-V& dI/dV curves for Antimony (Sb) doped two probe CNT system

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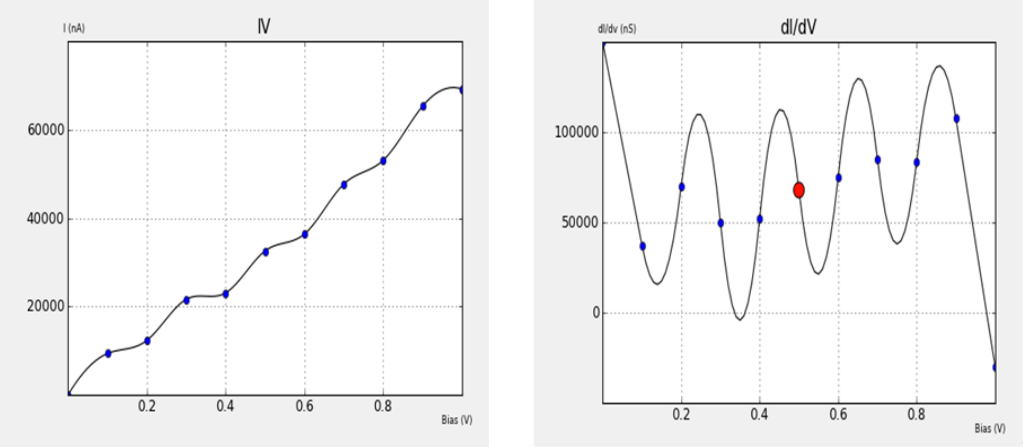

Figure 2(c): I-V& dI/dV curves for Arsenic (As) doped two probe CNT system

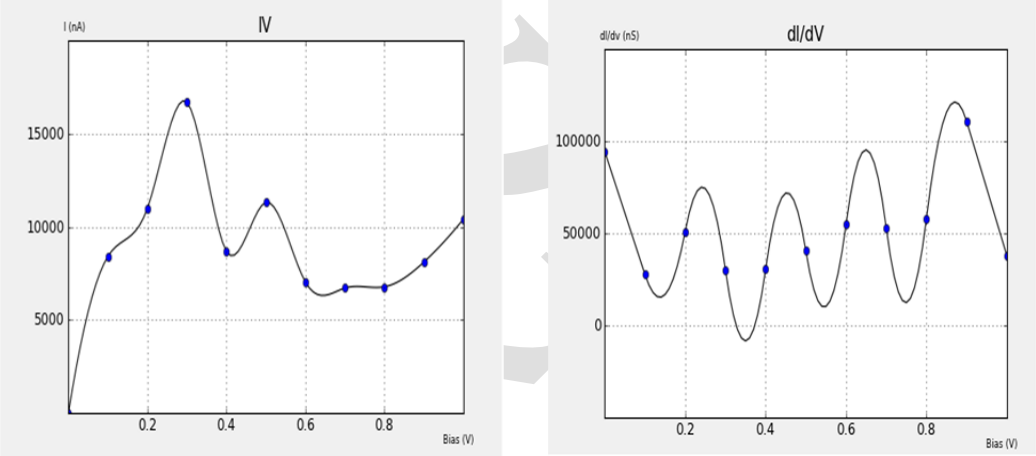

Figure 2(d): I-V& dI/dV curves for Chromium (Cr) doped two probe CNT system

Tellurium, Antimony & Arsenic are P-block elements and behave as donor impurity & therefore, it is expected that the influence of these dopants on the I-V characteristics and conductance will be greatly visible. In order to gain a clear picture we have introduced Table I & Table II. From Table II, it is clear that maximum conductance is shown by Arsenic doped two probe carbon nanotube system and minimum by Chromium. However, the chromium doped CNT device has shown an amazing property of NDR between 0.3-0.4 V & 0.5-0.6V as shown in Figure 2(d). NDR is a special property of some electric circuits and devices in which an increase in voltage across device terminals results in a decrease in electric current through it. This is in contrast to an ordinary resistor in which an increase of applied voltage causes a proportional increase in current due to ohm's law resulting in a positive resistance. While a positive resistance consumes power from current passing through it, a negative resistance produces power. Thus, it can increase the power of electric signal (amplification).

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TABLE 1: Values of current for two probe CNT system at different bias Voltages

APPLIED BIAS (V)	CURRENT (nA)			
	Tellurium	Antimony	Arsenic	Chromium
0	0	0	0	0
0.1	6092.18	9432.06	9552.83	8407.25
0.2	8520.13	12092.2	12308.6	10991.7
0.3	14828.5	21195.7	21620.4	16671.8
0.4	15279.8	22564.5	23041.7	8677.52
0.5	21251.1	32003.5	32539.9	11306.5
0.6	23523	35533.8	36343.4	7028.58
0.7	31672	46179.4	47665.3	6708.06
0.8	34347.5	52437.4	53020	6772.65
0.9	44878.3	64090	65274.2	8102.87
1.0	52304.5	69622.7	69750.7	10408

TABLE II: Values of conductance for two probe CNT system at different bias Voltages

APPLIED BIAS (V)	CONDUCTANCE (nS)			
	Tellurium	Antimony	Arsenic	Chromium
0	0	0	0	0
0.1	60921.8	94320.6	95528.3	84072.5
0.2	42600.65	60461	61543	54958.5
0.3	49428.33	70652.33	72068	55572.66
0.4	38199.5	56411.25	57604.25	21693.8
0.5	42502.2	64007	65079.8	22613
0.6	39205	59223	60572	11714.3
0.7	45246.71	65970.57	68093.28	9582.94
0.8	42934.375	65546.75	53020	8465.81
0.9	49864.77	71211.11	65274.2	9003.18
1.0	52304.5	69622.7	69750.7	10408

Figure 3, shows variation of conductance with applied voltage for two probe carbon nanotube system doped with atoms of Tellurium (Te), Antimony (Sb), Arsenic (As) & Chromium (Cr). Tellurium shows maximum conductivity of 60921.8nS at bias voltage of 0.1V. Thereafter, the conductivity shows terracing slopes. Antimony and Arsenic dopants have almost increased the conductance in equal proportions but Arsenic dopants has sustained maximum conductivity over a wide range of applied bias voltages as shown in Figure 3. The maximum conductivity in Antimony & Arsenic doped CNT is 94320.6nS & 95528.3nS respectively. Therefore, Arsenic doped CNT enhanced conductivity due to the maximum modulation in Fermi level when compared with other dopants. In contrast, Chromium is showing maximum

ISSN: 2319-8753

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conductivity of 84072.5nS. As the applied bias is increased in chromium doped CNT multiple negative differential resistance is reported between 0.3-0.4V & 0.5-0.6V

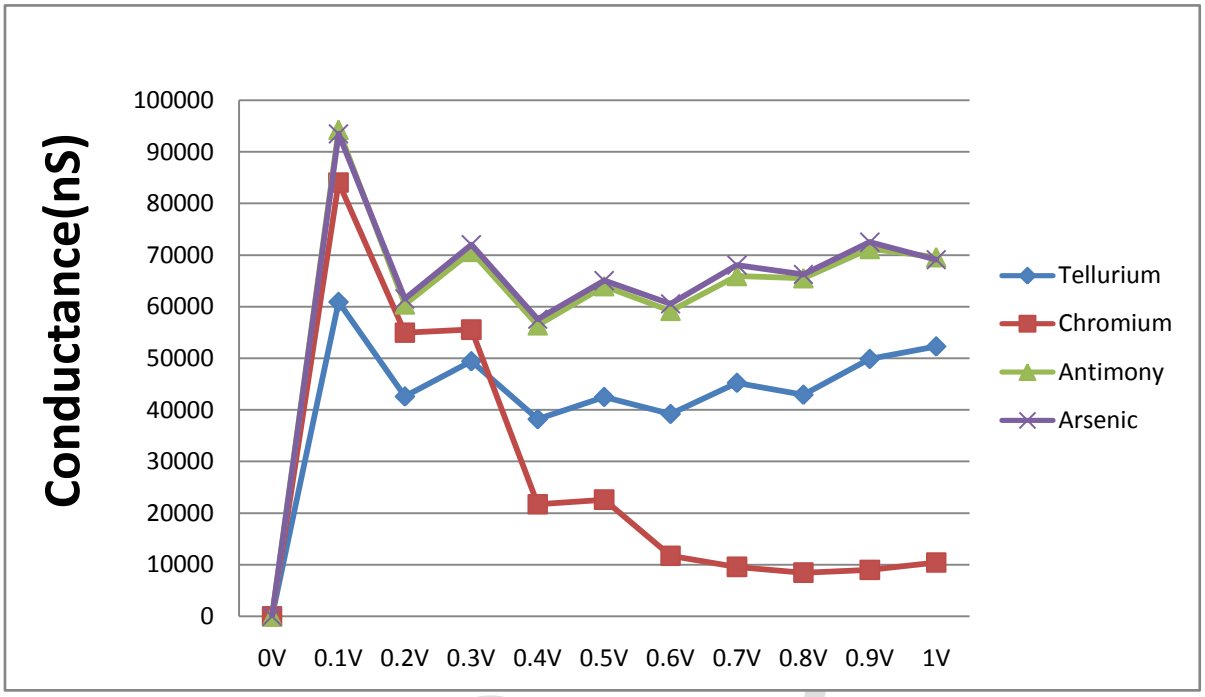

Figure 3: Conductance Vs Voltage graph showing doping effects on two probe CNT system.

V. CONCLUSION

In this paper, we have successfully simulated the Zig-Zag (4, 0) single walled carbon nanotube with different dopants using ATK 13.8.1. The results show that all the device models show different conductivity behavior at different bias voltages. The maximum conductivity was reported in Arsenic whereas multiple negative differential resistance was shown in chromium doped CNT. These results indicate that doping can modulate the electrical transport properties of carbon nanotubes, however, the electronic device transport properties are dependent on position, number and type of dopants. Moreover, the effect of doping on the transport properties of carbon nanotubes is generally attributed to the modulation in Fermi level. The increase in conductance shown by Arsenic doped carbon nanotubes is important for the design of carbon nanotube based high speed arthimatic architectures such as Adders, Multipliers etc whereas Chromium doped CNT is suitable for CNT based nanodevices such as amplifiers, oscillators and is particularly suitable for microwave frequency operations.

ACKNOWLEGEMENT

The authors greatly acknowledge the financial support by University Grants Commission (UGC), New Delhi (grant F-No: 42-768/2013) which enables this study to occur.

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