Modeling the Conductivity Enhancement in Doped Single- walled Carbon Nanotube (SWCNT)

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ABSTRACT

Abstract: In this work we have modeled and simulated the electronic charge transport properties for a Single-walled Carbon Nano-tube with different geometries using first-principle calculations and Nonequilibrium Green's function (NEGF) method. We modeled a Single-walled Carbon Nano-tube by rolling Armchair (4,4) or Zigzag (4,0) Graphene Nanoribbon strips with the different doping atoms (S,N,P) using semi-empirical Extended Huckle Theory (EHT) within the framework of non-equilibrium green function (NEGF). The simulations were carried in Device mode using Atomistic Tool Kit (ATK-12.8.2) and its graphical interface (custom analyzer) Virtual Nano Lab till the self-consistent results was reached. The effect of the change in conductance and I-V characteristics of the junction was visualized for various transport parameters. The distinct changes in conductance reported as the positions , concentration and type of dopants was varied in central region of the CNT between two electrodes at different bias voltages from -2V to 2 V with steps of .50 V. This suggested conductance enhancement mechanism for the charge transport in the doped Single-walled Carbon Nano-tube at different positions is important for the design of CNT based nano electronic devices.

Keywords: Electronic charge Transport, Extended Huckle Theory (EHT), NEGF, SWCNT, Dopants ,GNRs , Atomistic Tool Kit (ATK-12.8.2)

INTRODUCTION

Carbon Nanotubes (CNTs) are very attracting since they had been discovered in 1991 by Iijima [1] due to their excellent mechanical behavior and due to electrical and thermal properties. Their name is driven from their long, hollow structure with the walls formed by one-atom-thick sheets of carbon i.e graphene. Nanotubes are of two types single-walled and multi- walled nanotubes having chiral, zigzag and armchair geometries. The CNTa can be metallic or semiconducting, depending on their chirality. The physical, chemical, electrical and optical properties of any solid can be determined by its quantized electronic states. These quantum states in nano-scale systems are produced due to the confinement of the carrier charges in one or two dimensions.

Carbon nanotubes can serve as an excellent media to address some mesocsopic phenomena related to size effects like Coulomb-blockade ,Ballistic transport , super current and universal conductance fluctuation [2-3]. However the nano-scale size of the carbon naotubes makes it extremely difficult to study the physical properties on a single carbon nanotube. It is necessary to further address whether the transport of the CNTs is controlled by ballistic or diffusive mechanism and how the doping effects the electrical properties of the CNTs, which is very important in the band-gap design engineering to make a real molecular –level single electron device. The electronic transport properties for CNTs are investigated by applying Non-equilibrium Green's functions in combination with the first-principles theory. The position, number and type of the dopants are varied randomly in the central region of the CNT between two electrodes.

DESCRIPTION & SIMULATIONS for the MODEL

We modeled a Single-walled Carbon Nano-tube (SWCNT) by rolling Armchair (4, 4) or Zigzag (4,0) Graphene Nanoribbon strips with the different doping atoms (S,N,P) and configured the setup for device mode as shown in the figure 1.

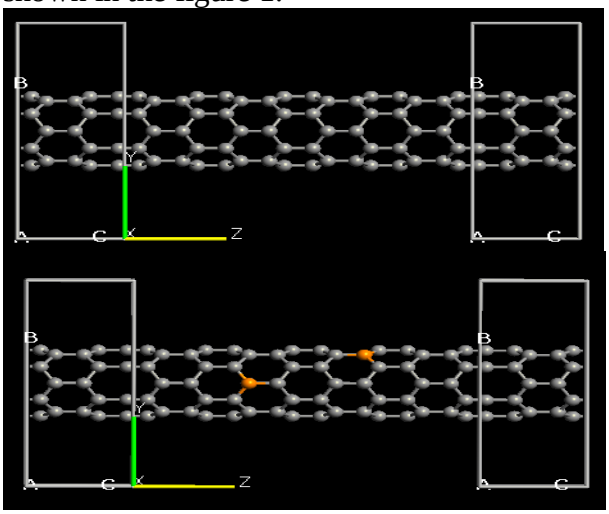

Figure-1) Model of Pure and doped CNT coupled with Left (L) and Right (R) electrodes in device mode.

The device mode consists three parts, i.e. left electrode, scattering region and right electrode. Both electrodes are semi-infinite CNTs and scattering regions are composed of doped CNTs. The carbon-carbon bond length was selected as 1.42086 Å and the length of the two electrodes was considered to be 5.52516 Å for the better geometry optimization. 25% of the length of the electrodes (1.38129 Å) was considered as the central molecule along with the central region in order to compensate for the 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 CNT inserted between two semi-infinite electrodes to predict the electron transport through the junction under varying conditions of bias voltages. The hypothesis for this electron transport was based on Non-equilibrium green function (NEGF) formulism [4]. We implemented semi-empirical Extended Huckle Theory (EHT) device mode approach [5], the results produced using this approach are in near approximation to the results produced using experimental techniques. We assumed in this work that, under the simulated conditions, inelastic scattering processes were negligible and thus we were dealing with an effectively ballistic transport regime. We adopted the single-particle approach to transport modeling, which is based on the Landauer-Buttiker formalism, and still allowed for elastic scattering from macroscopic potentials.

For producing real time scattering effects, we considered Cerda Huckle parameters i.e. Cerda carbon and Cerda hydrogen with vacuum level of -7.36577eV & -6.2568eV respectively [6]. The grid cut-off was considered to be 10 Hartrees, Maximum Interaction range 10Å, while k-point sampling was taken (2, 2,100) for the calculation to be optimal combination of accuracy and speed. We adopted FastFourier2DSolver as tool for Poisson solver of the boundary conditions. Monkhorst Pack Grid (1, 1) at average Fermi level was enforced under self-consistent measurement to calculate the density matrix. Once the calculation of density matrix was completed, the Fermi level is computed. This Fermi level was the default electrode potential of the right electrode. Depending upon the applied bias at the left electrode, the electrode potential of the left electrode was calculated. The electron temperature was set at 300K for all simulations, before the geometry optimization was done. We varied the applied bias across the two electrodes in the range of --2 Volts to 2 Volt in the steps of 0.5 V and measured the effective variation in the values of current and conductance.

THEORY of THE MODEL

According to the transport theory in low-dimensional systems , the quntum step behaviour in transport of CNT was attributed to the two conducting transverse modes ($2G_o$) where $G_o = 2e^2/h$ [7-9] .The current was calculated by the Landauer–Buttiker formula [10-11] which gives the conductance of the low dimensional system in terms of the Electron Transmission Coefficient represented as $G = \frac{2e^2}{h} T(E,Vb)$

Where h is the Planck constant and T(E,Vb) is the Transmission coefficient from left to right electrode expressed as

$T(E,Vb) = Tr(\Gamma_R G_C^R \Gamma_L G_C^A)$ where G_C^R , G_C^A are the retarded and advanced Green's functions of the conductor and Γ_L is the coupling matrices from conductor to the left electrode. Within the NEGF formalism [12]

$$\Gamma_L = i\,[\in_L - \in_L^{\dagger}]$$

and $\Gamma_R = i\,[\in_R - \in_R^{\dagger}]$

where $\in_L, \in_R$ are the self-energies.

$$I = \frac{2e^2}{h}\int T(E,V_b)[f_l(E) - f_r(E)]dE$$

Or

$$I = \frac{1}{e}\int_{-\infty}^{\infty} d\varepsilon[n_F(\varepsilon - \mu_L) - n_F(\varepsilon - \mu_R)G]$$

Where μ_L and μ_R are the electromechanical potentials of the left and right electrode, respectively.

RESULT AND DISCUSSION

For the above said device model shown in figure-1 the transmission spectrum *T*(*E; V*b) with 200 point in the energy range [-2,2] eV , Electron Difference Density, Electrostatic Difference potential and Device Density of states (DOS) was calculated using Atomistic Tool Kit (ATK-12.8.2) at different bias voltages [13]. Then the position, concentration and type of dopant is varied in the central region at the fixed electron temperature. Again the transmission spectrum *T*(*E; V*b) with 200 point in the energy range [-2,2] eV , Electron Difference Density, Electrostatic Difference potential and Device Density of states (DOS) was calculated at different bias voltages across the two electrodes. The transmission spectrum for all simulations was analyzed in the custom analyzer of Virtual Nano Lab (ATK-12.8.2) by plotting I-V and Conductance curves with respect to different applied bias voltages. The figure 2 shows the I-V & dI/dV-Vcurves and figure 3 shows the quantum conductance & transmission spectra curves for the pure CNT as well as 2 atoms doped CNT with Nitrogen, Phosphorus & Sulfur dopants.

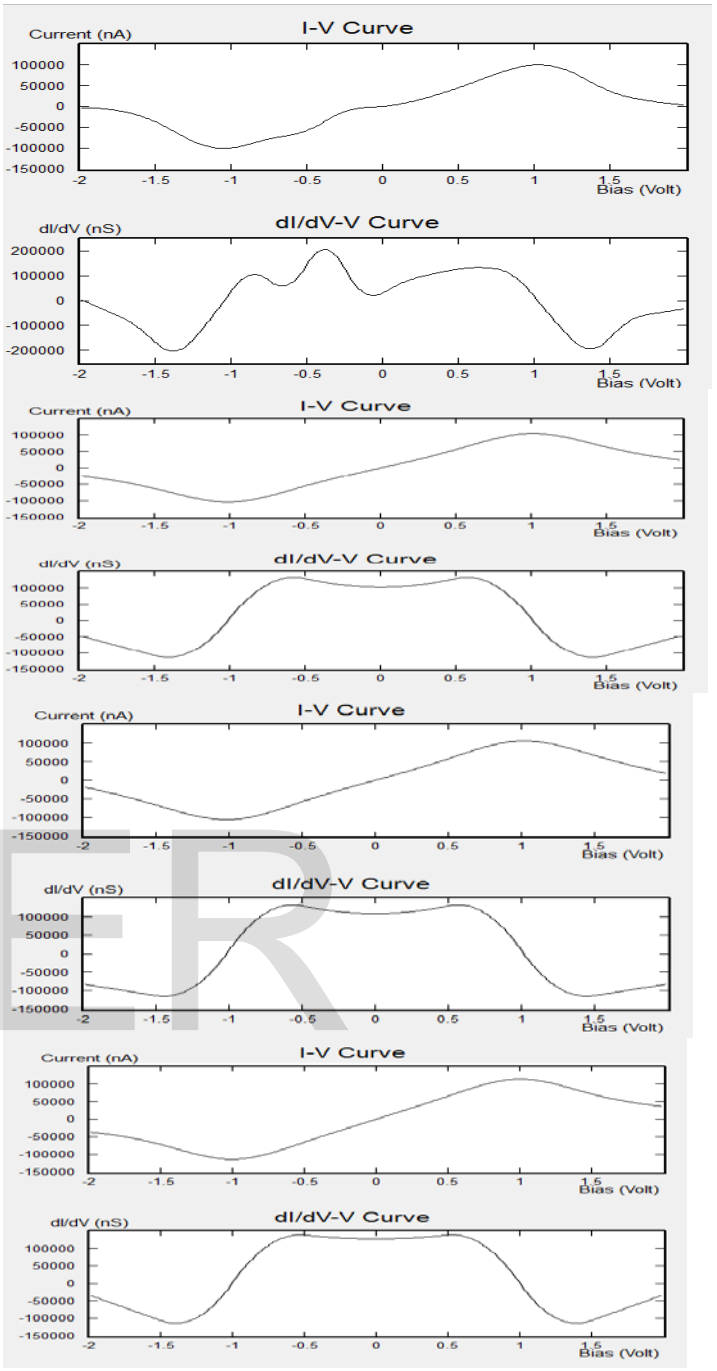

Figure-2) The I-V & dI/dV-Vcurves for Pure and N, P, S doped CNTs.

The negative differential resistance (NDR) region reported ie. exhibit NDR behaviors, with dips in the current values with rise in the voltages for positive bias.

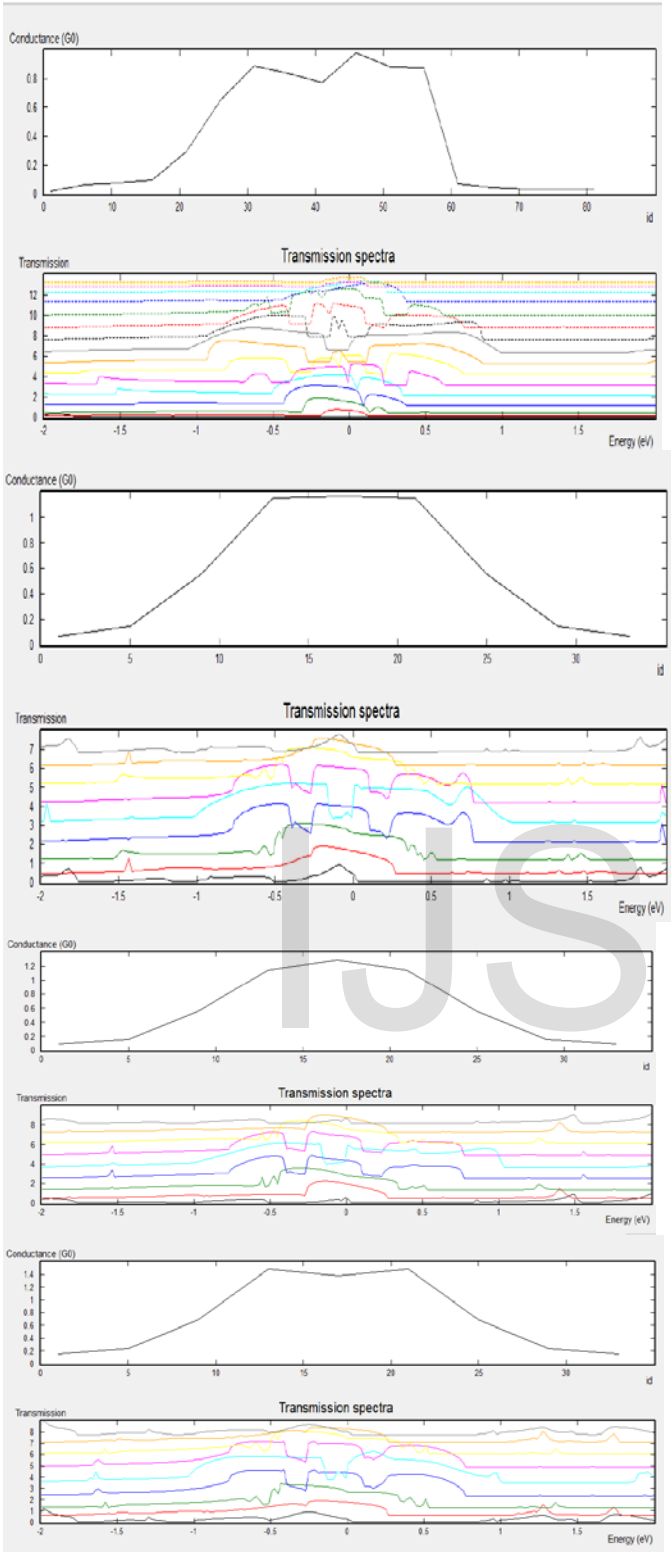

Figure-3) The Quantum Conductance & transmission spectra curves for Pure and N, P, S doped CNTs.

After the analysis we find the all the dopants shows different transport behaviors. The maximum conductivity enhances upto 10^{-3} S by doping the sulfur atoms whereas the normal maximum conductivity reported in the range of 10^{-5} S. Hence the current and conductance through doped CNTs varies substantially with the increase of the bias voltage from -2 V to 2 V.

CONCLUSIONS

The simulated results show that the electronic transport properties of doped CNTs can be varied at different bias voltages. So doping can modulate the electrical transport properties of CNTs. The electronic transport property depends on position, number and type of dopants for different bias voltages at constant electron temperature. The effect of doping on transport behavior can be attributed to the modulation to the Fermi level by the Doped CNTs. This suggested conductance enhancement and NDR mechanism for the charge transport in the doped Single-walled Carbon Nano-tube at different positions is important for the design of CNT based nano electronic devices.

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