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Modeling the Effect of Charge Transport in Graphene Nano Ribbons with Doping Concentration

Ravinder Kumar[1*], Harpinder Kaur [1] , Vijay Lamba[2] , Derick Engles[1]

[1]Department of Electronics Technology
Guru Nanak Dev University, Amritsar (PUNJAB), India- 143005
[2]*Global College of Engineering & Technology, Khanpur Khui*

ABSTRACT

In this work, we scrutinized the effect of doping on current and conductance by varying the percentage number of dopants in the different geometries of Graphene Nano Ribbon (GNR). We modeled and simulated the Armchair (4, 4) & Zigzag (4, 0) Graphene Nanoribbon strips with different number of dopant atoms in two probe system 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-12.8.0) and its graphical interface (custom analyzer) Virtual Nano Lab till the self-consistent results was reached. The distinct changes in conductance , I-V curves and NDR behavior reported as the number of dopant atoms and position of the dopant was varied at different bias voltage (-2 to 2V) with steps of .50 V and constant electron temperature. This suggested conductance controlled mechanism for the charge transport in the GNRs is important for the design of graphene based nano electronic devices.

Keywords: Grephene Nano Ribbon, Dopants, EHT, NEGF, Atomistic Tool Kit (ATK-12.8.0).

INTRODUCTION

Graphene nanoribbons are among the recently discovered carbon nanostructures, with unique characteristics for novel basic science and application points of view, is their electrical conductivity. Graphene nanoribbons (GNRs) have attracted intensive interest because of their unique electronic properties and vast potential for device applications. In particular, the GNR based devices could behave like molecule devices, such as those based on carbon nanotubes (CNTs) but with some inherent advantages, including more straightforward fabrication processes by using lithography technique and better control of crystallographic orientation in constructing device junctions. Different from CNTs, the existence of edge structures endows GNR with some novel physical and chemical properties, such as the high edge reactivity and unique edge states around the Fermi level. These may offer key advantages in realizing various electronics applications via edge chemical functionalization, such as doping.

The well-known dopants are like Nitrogen (N) , Sulfur (S) , Phosphorus (P) atoms are typical substitutional dopants in carbon materials (like GNRs & CNTs), and their binding with the C atom is covalent and quite strong, comparable to that of host C-C bond. Our model is based on the incorporation of N or B atoms into the carbon materials which will influence the electronic and transport properties of the C host by introducing extra carries and/or new scattering centers.

DESCRIPTION & SIMULATIONS of the MODEL

We modeled and simulated the Armchair (4, 4) & Zigzag (4, 0) Graphene Nanoribbon strips with different number of dopant atoms in two probe system shown in figure 1, using semi-empirical Extended Huckle Theory (EHT) within the framework of non-equilibrium green function (NEGF).

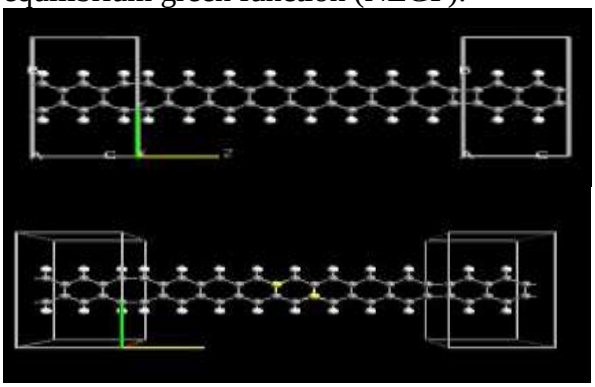


Figure1. Device Model for Zig-Zag pure and doped ZNR.

The quantum transport calculations were performed using the Atomistix Tool Kit (ATK-12.8.0) in Device mode and its graphical interface (custom analyzer) Virtual Nano Lab till the self-consistent results was reached. The device mode consists three parts, i.e. left electrode, scattering region and right electrode. Both electrodes are semi-infinite GNRs and scattering regions are composed of different doped configurations of the GNR. The carbon-carbon bond length was selected as 1.42086 Å and the length of the two electrodes was considered to be 6.3830 Å for the better geometry optimization. 22% of the length of the electrodes (1.43043 Å) was considered as the central molecule along with the GNR in order to compensate for the scattering losses at the joining ends of the central molecule and the left-right electrodes. The hypothesis for this electron transport was based on Non-equilibrium green function (NEGF) formulism. We implemented semi-empirical Extended Huckle Theory (EHT) device mode approach, 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. 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 300 K for all simulations, before the geometry optimization was done. We varied the concentration of the dopants in GNR geometries with fixed temperature and different applied bias across the two electrodes in the range of -2 Volts to 2 Volt in the steps of 0..50 V and measured the effective variation in the value of current and conductance.

THEORY of THE MODEL

Landauer's Formula is normally used in order to compute current in nanoscale devices. Electric current flow is often viewed as an electron (or charged carriers) response to an applied electric field. Landauer viewed current flow as a transmission process, or a consequence of the injection of carriers at contacts and probability of the carriers to reach the other end. This approach has proven to be extremely useful for transport properties of nanostructured materials and devices, including molecular systems. Landauer's original result was obtained for a system of two one-dimensional leads connecting to a sample. The two leads are connected to two macroscopic electrodes or electron reservoirs. The sample is where scattering can take place and characterized by a transmission function *T(E,V)*. The conductance *C (E,V)* of the system is given by

$$C(E,V) = G = \frac{2e^2}{h} T\,(E,V)$$

where e is the electron charge, *h* is the Planck constant, and *T(E,V)* is the transmission probability.

A closely related method is the non-equilibrium Green function method. The non-equilibrium Green's function method has important applications within solid state, nuclear and plasma physics. However, due to its general nature it can equally deal with molecular system. The method has as its main ingredient the Green function, which is a function of two space-time coordinates. From knowledge of this function one can calculate time dependent expectation values such as currents and densities, electron addition and removal energies and the total energy of the system. In the absence of external fields the non-equilibrium Green function method reduces to the equilibrium Green function method which has had imporatnt applications in quantum chemistry. Green function is also used in the transport calculation of graphene Nano ribbons

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

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 . Then these strips were doped with 1, 2, 3 number of different dopant atoms (like B,N,S,P) and 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-12.8.0) by plotting

I-V curves shown in the figure -2 and dI/dV-V curves shown in the figure-3. By analyzing the results we reported a decrease conductance with addition of the doping atoms.

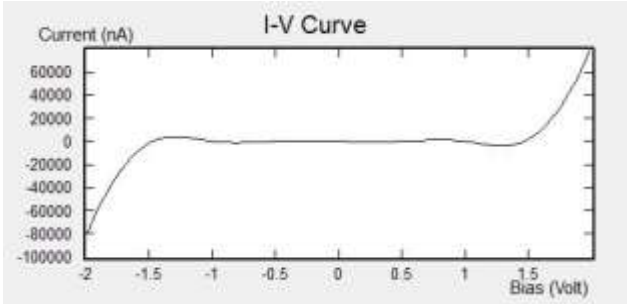
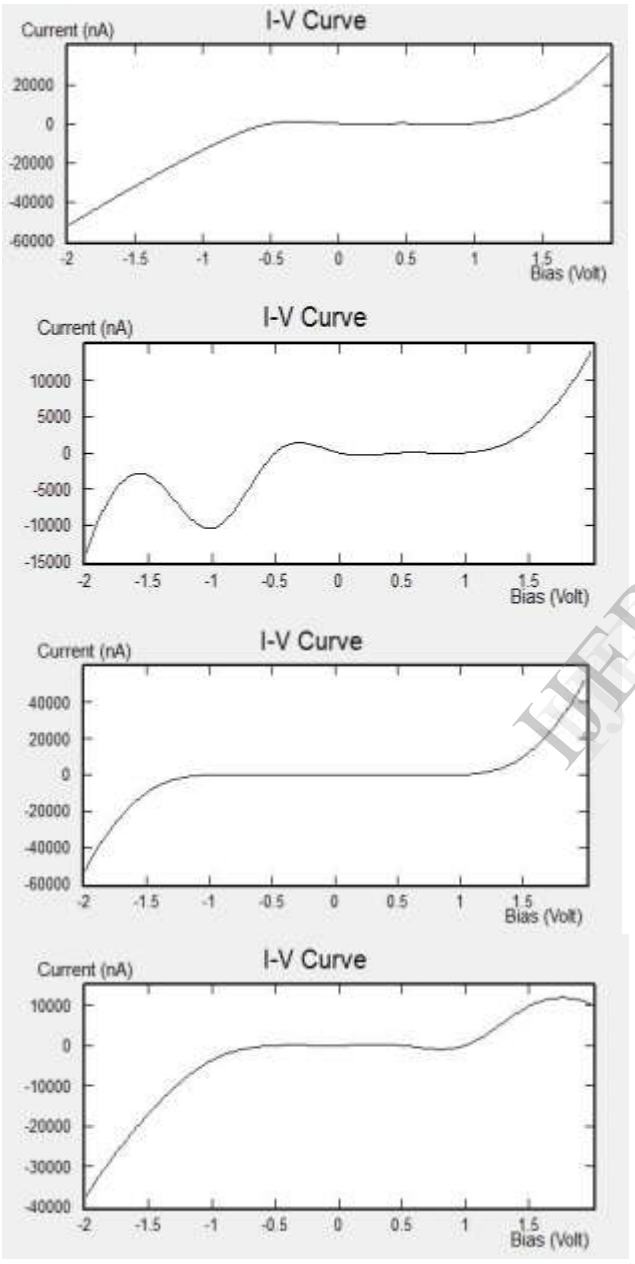
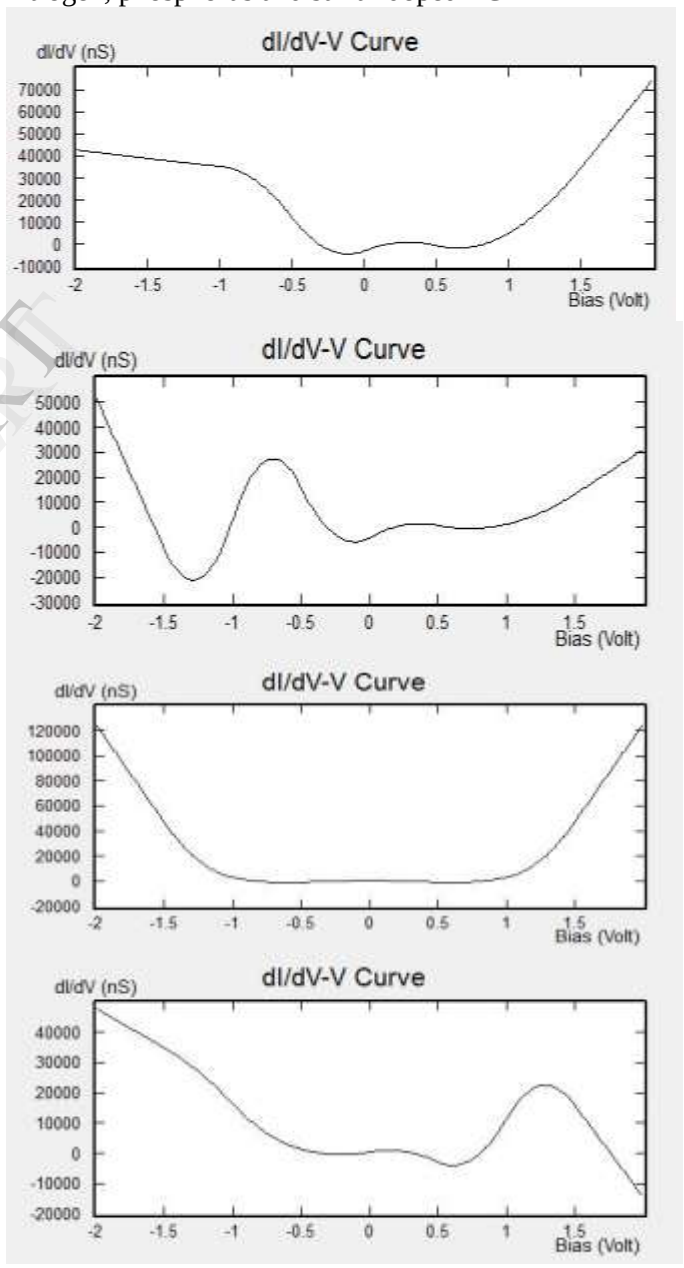


Figure 2. I-V curves for pure, 2-atoms boron, nitrogen, phosphorus and sulfur doped ZGNR





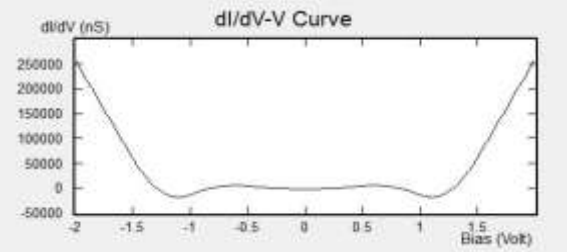


Figure 3. dI/dV-V Curves for 2-atoms boron, nitrogen, phosphorus and sulfur doped ZGNR.

CONCLUSIONS

The simulated results show that the current and conductivity decreases when we increase the number of doping element (B, N, S, and P) in different GNR geometries. The conductance can be controlled only up to certain concentration level because more number of dopants can destroy the Nano structural geometries. The negative differential resistance (NDR) region reported with the doping of Sulfur or Phosphorus atoms ie. exhibit NDR behaviors, with dips in the current values with rise in the voltages for positive bias. This suggested conductance controlled mechanism for the charge transport in the GNRs is important for the design of graphene based nano electronic devices.

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