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Analytical quantum current modeling in GNSFET

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ABSTRACT: Carbon nanoscrolls (CNSs) belong to the same class of carbon-based nanomaterials as carbon nanotubes. As a new category of quasi one dimensional material Graphene Nanoscroll (GNS) has captivated the researchers recently because of its exceptional electronic properties like having large carrier mobility. GNS shape has open edges and no caps unlike Single Wall Nanotubes (SWNTs) which are wound into close cylinders' shape. The carbon atoms on the edge of GNS have two typical topological shapes. GNS can be classified to either AGNS or ZGNS according to its topological structure. However, in this research, only ZGNS was taken into consideration because AGNS behaves as metallic unlike ZGNS which can behave either metallic or semiconducting depends on their chirality which is the main highlight in this project. In this project, the modeling of GNS was done and their electrical characteristic and behavior were investigated. Also by utilizing analytical approach, introduces modeling the quantum current for graphene nanoscroll Furthermore.

Keywords: *Armchair GNS, Fermi-Dirac integral, Graphene Nanoscroll, Quantum Current, Zigzag GNS.*

INTRODUCTION

Carbon nanoscrolls (CNSs) belong to the same class of carbon-based nanomaterial as carbon nanotubes but are much less studied in spite of their great potential for applications in nanotechnology and bioengineering. As shown in Fig. 1, GNS are the jelly roll-like wrapping of a graphite sheet to form a nanotube [1]. GNS has the ability to control the length of the overlapping region thus make them possess great electrical and electronic properties [2]. GNS exhibits different electronic properties depending on their chirality. Chirality defined as the circumference of GNS. With the band gap, they can behave as metallic or semiconducting depending on their chirality. GNS is formed by rolling up a single layer of graphene. GNS shape has open edges and no caps unlike Single Wall Nanotubes (SWNTs) which are wound into close cylinders' shape. The carbon atoms on the edge of GNS have two typical topological shapes. GNS is a 1D structure with the confinement of carriers in two directions. The direction of the roll-up is specified by the chiral vector [3].

GNS is classified according to their chirality. The chirality which is represented by the chiral vector has two typical shapes, namely zigzag and armchair GNS [4]. The type of GNS depends on the chiral vector that is if the chiral vector lies along the x-axis, it is known as an armchair GNS and if the chiral vector lies along the

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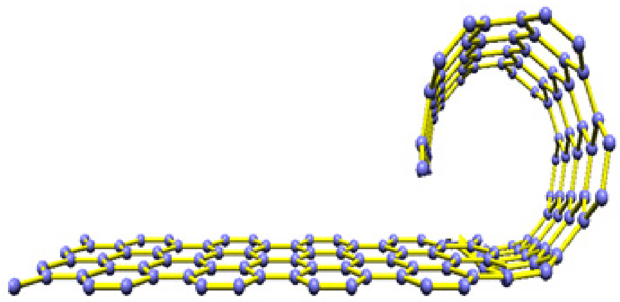

Fig. 1. Graphene Nanoscroll geometries.

y-axis, it is known as a zigzag GNS. The notation of Armchair GNS (AGNS) is given by [n, n] while zigzag GNS (ZGNS) can be represents by [n, -n] or it also be known as [n, 0]. AGNS behaves as metallic while ZGNS can behave whether metallic or semiconducting depends on the number of chirality. Chirality also affects the band structure, DOS, and carrier concentration of GNS. On the other hand, the current in the channel of GNSFET is varied caused by the different number of chirality. The structure of GNSFET is similar to the conventional MOSFET where it has gate terminal, drain terminal, source terminal, and conducting channel. Fig. 2, shows the structure of GNSFET [5,6]. The structure is no different as CNTFET as GNS replace CNT as the material to form GNSFET.

MATERIAL AND METHODS

The basic step in GNS modeling is the energy spectrum E (k) of a graphene. Generally, tight binding energy dispersion is applied to obtain the band gap in GNS. The general equation of band structure is based on the energy band throughout the entire Brillouin zone of graphene is shown in the equation (1) below.

$$\vec{E}(\vec{k}) = \pm t\sqrt{1+4\cos\left(\frac{3}{2}k_x a_{cc}\right)\cos\left(\frac{\sqrt{3}}{2}k_y a_{cc}\right)+4\cos^2\left(\frac{\sqrt{3}}{2}k_y a_{cc}\right)} \quad (1)$$

Where $k_{x,y,z}$ is wave vector component, t=2.7 (eV) is the nearest neighbor C-C bonding energy and is Carbon-Carbon (C-C) bond length. The positive sign indicates the conduction band while valence band is given by negative sign. The equation was simulated by using MATLAB and the result obtained is shown in Fig. 3.

Fig. 3, shows the throughout the entire Brillouin zone of graphene and also known as non-parabolic energy band diagram. It shows the presence of energy band gap between the conduction band and valence band. Therefore, it can be concluded that ZGNS behaves as semiconducting material. In GNS the chiral vector ($\vec{C}$) determines the direction of the roll-up $\vec{C}=n\vec{a}_1+m\vec{a}_2$ where, $\vec{a}_1=3/2a_{cc}\vec{i}+\sqrt{3}/2a_{cc}\vec{j}$, $\vec{a}_2=3/2a_{cc}\vec{i}-\sqrt{3}/2a_{cc}\vec{j}$ and where the integers (n) and (m) are the number of steps along the unit vectors $\vec{a}_1$ and $\vec{a}_2$. It is possible for us to have an armchair nanoscroll if $\vec{C}$ lies along the x-axis whereas a zigzag nanoscroll if $\vec{C}$ lies along the y-axis. Vector of T is the translational vector along the nanoscroll axis [7-9]. Consequently, in zigzag graphene nanoscroll whose circumferential direction is around the y-axis, the energy dispersion relation utilizing the tight binding model and enforcing boundary condition $\vec{k}.\vec{C}=L$ is determined as;

$$\vec{E}(\vec{k}) = \pm t\sqrt{1+4\cos\left(\frac{3}{2}k_t a_{cc}\right)\cos\left(\frac{L}{2n}\right)+4\cos^2\left(\frac{L}{2n}\right)} \quad (2)$$

Where $\vec{k}$(the wave vector) can be obtained by $\vec{k}=k_x i +$

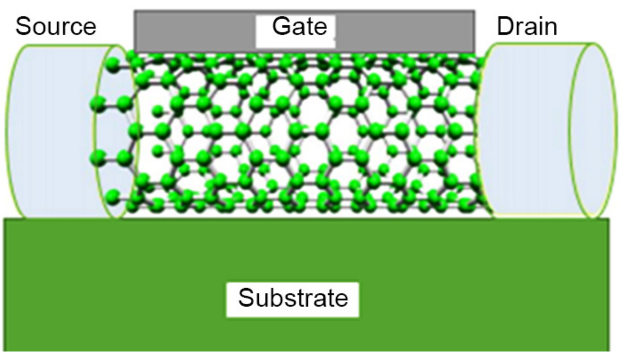

Fig. 2. Structure of GNSFET.

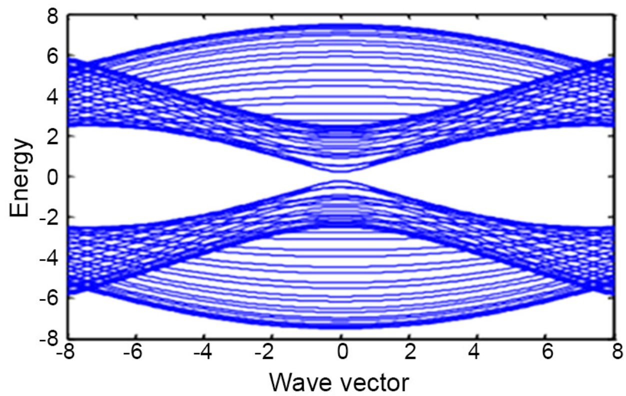

Fig. 3. A Band structure of GNSs for different values of k.

$k_y j$, $\vec{k}_t$ denotes the k's magnitude along the axis of the nanoscroll and the range of $\vec{k}_t$ will be $-2\pi/3a_{cc} \leq \vec{k}_t \leq 2\pi/3a_{cc}$, While a_{cc}=1.42°A will be the carbon-carbon bonding distance or the length of the carbon-carbon atom and (t = 2.7ev) stands as the closest neighbor C-C overlap energy while (n) signifies the chirality number. Furthermore, by utilizing the equation of the energy dispersion, k can be acquired as:

$$\vec{k} = \pm \frac{\sqrt{m^*}}{3\hbar\sqrt{t}}\left(E - E_c\right)^{\frac{1}{2}} \quad (3)$$

As a result, energy is equal to;

$$E = \frac{9\hbar^2 k^2 t}{m^*} + E_c \rightarrow E = \frac{9\hbar^2 k^2 t}{m^*} + \frac{1}{2}t + \frac{3L^2}{2n^2} \quad (4)$$

Energy changes equal to;

$$\Delta E = \frac{6\hbar\sqrt{t}}{\sqrt{m^*}}\left(E - E_c\right)^{\frac{1}{2}} \Delta k \quad (5)$$

Where m^* provided by Equation (4) can be considered as the efficient electron mass in the ZGNS and t is the closest neighbor C-C overlap energy, E_c denotes the energy of the conductance band derived as $E_c=1/2t+3L^2/2n^2$, L shows the length of the spiral in GNS and n stands for the chirality.

RESULT AND DISCUSSION

In GNSs the current from source (S) to drain (D) given by the Boltzmann transport equation is [9].

$$I = \frac{2q}{h}\int_{E_{f1}}^{E_{f2}} Dos(E)T(E)\left(-\frac{df}{dE}\right)dE \quad (6)$$

Where, q is the electron charge, h is Planck's constant, EF1 and EF2 are the Fermi levels of Source and Drain, Dos (E) is Density of States; T(E) is the transmission probability and $f(E)=1/1+e^{E-Ef/KaT}$ is the Fermi function. Therefore, at the beginning for the modeling of current we start by the modeling of the Dos (E) which is presented for the zigzag nanoscroll. Because of the structure of the ZGNS is a confined one-dimensional (1D) structure, the Dos (E) (normalized per unit length) for ZGNS can be obtained through [10]:

$$Dos(E) = \frac{\Delta n}{l\Delta E}, \Delta k = \frac{2\pi}{l}\Delta n, Dos(E) = \frac{\sqrt{m^*}}{12\pi\hbar\sqrt{t}}\left(E - E_c\right)^{-\frac{1}{2}} \quad (7)$$

High carrier mobility reported from experiments in the graphene leads to assume a completely ballistic carrier transportation in the graphene, which implies that average probability of injected electron at one end transmitting to the other end is approximately equal to one (T(E) =1). In practice, by incorporating and integrating the Fermi-Dirac distribution function against the energy, the sum of the current within a band can be acquired. Accordingly, the current can,

$$I = \frac{2q}{h}\int_{E_{f1}}^{E_{f2}} \frac{\sqrt{m^*}}{12\pi\hbar\sqrt{t}}\left(E - E_c\right)^{-\frac{1}{2}}\left(-\frac{d\left(\frac{1}{1+e^{\frac{E-E_f}{K_B T}}}\right)}{dE}\right)dE \quad (8)$$

or

$$I = \frac{2q}{h}\int_{E_{f1}}^{E_{f2}} \frac{\sqrt{m^*}}{12\pi\hbar\sqrt{t}}\left(E - E_c\right)^{-\frac{1}{2}}\left(\frac{1}{K_B T}\right)\left(\frac{e^{\frac{E-E_f}{K_B T}}}{\left(1+e^{\frac{E-E_f}{K_B T}}\right)^2}\right)dE \quad (9)$$

Finally, the current based on the Fermi-Dirac integral is as follows,

$$I = \frac{q\sqrt{m^*}}{12\pi^2\hbar^2\sqrt{K_B T t}}\int_0^{\eta} x^{-\frac{1}{2}} \frac{e^{x-\eta}}{\left(1+e^{x-\eta}\right)^2}dx \quad (10)$$

The study of the current-voltage response of an electronic device is one of the main topics in electronics. By replacing $\eta \approx V_{GS}-V_T/k_B T/q$ in equation (10), the current-voltage relationship of GNS can be gained from equation (11),

$$I = \frac{q\sqrt{m^*}}{12\pi^2\hbar^2\sqrt{K_B T t}}\int_0^{\eta} x^{-\frac{1}{2}} \frac{e^{x-\frac{q(V_{GS}-V_T)}{k_B T}}}{\left(1+e^{x-\frac{q(V_{GS}-V_T)}{k_B T}}\right)^2}dx \quad (11)$$

The drain current in GNS FETs depends on the gate voltages. The source- drain current is due to the applied voltage dependences of the potential distributions along the channel. The obtained analytical formulas for the source-drain current can be used for GNS-FET optimization by the proper choice of the thicknesses of gate layers, the top-gate length, and the bias voltages. Fig. 4, shows current model in GNS

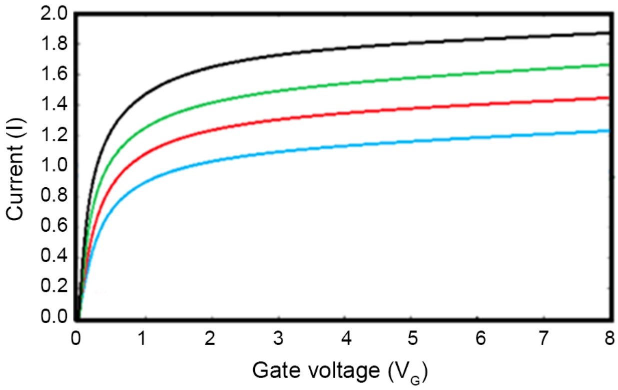

Fig. 4. The Current (I) variation of GNS as a function of the Gate Voltage (VG).

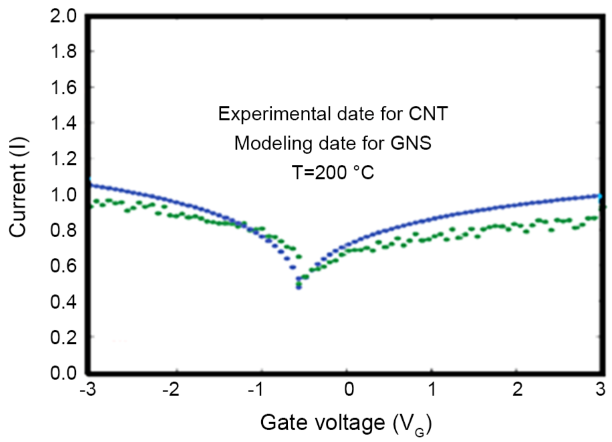

Fig. 5. I-V characteristics of the GNS (blue point), compared with the experimental data of the CNT (green point) at T=200 °C.

based on equation (11) where Fermi-Dirac distribution function has been approximated by Maxwell-Boltzmann distribution function.

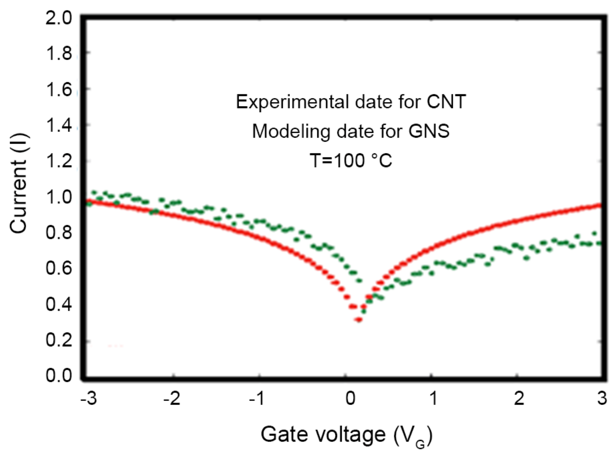

Fig. 6. I-V characteristics of the GNS (blue point), compared with the experimental data of the CNT (green point) at T=100 °C.

Also the current in GNS FETs depends on the temperature. Fig. 6, and Fig. 7, shows the representative current–voltage (I-V) characteristics at different temperatures (T=100 °C and T=200 °C). The nonlinear behavior of current–voltage characteristics at low threshold, and the second ohmic region in the strong electric field can be explained by the heating effect. Within a strong electric field, the current grows sharply with heating. At sufficiently high electric field, we observe linear I-V over the whole temperature measurement range. Also, the results compared with experimental data and there is good agreement between results and experimental data.

CONCLUSIONS

There are a lot of possibilities for the research in this field since the field study of GNS is very new and many researchers show their interest towards it. The research is endless and GNS gives bright future for nanoscale device technology. The different chirality of the GNS which is the main topic in this research that affect the electrical properties of the GNSFET will also be discussed. In this project, the modeling of GNS was done and their electrical characteristic and behavior were investigated. Also by utilizing analytical approach, introduces modeling the quantum current for graphene nanoscroll Furthermore. Finally, comparison with experimental data will show the validity of the GNSFET model.

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REFERENCES

[1] Pan, H., Feng, Y. and Lin, J. (2005). An initio study of electronic and optical properties of mul-

tiwall carbon nanotube structures made up of a single rolled-up graphite sheet. Physical Review B, 72, 085415.

[2] Shioyama, H. and Akita, T. (2003). A new route to carbon nanotubes. Carbon, 41, 179-181.

[3] Mpourmpakis, G., Tylianakis, E. and Froudakis, G.E. (2007). Carbon nanoscrolls: a promising material for hydrogen storage. Nano Letters, 7, 1893-1897.

[4] Xie, X., Ju, L., Feng, X.F., Sun, Y.H., Zhou, R.F., Liu, K., Fan, S.S., Li, Q.L. and Jiang, K.L. (2009). Controlled fabrication of high-quality carbon nanoscrolls from monolayer graphene. Nano Letters, 9, 2565-2570.

[5] Akhmerov, A.R., Bardarson, J.H. Rycerz, A., Beenakker, C.W.J. (2008). Theory of the valley-valve effect in graphene nanoribbons. Physical Review B, 77 (20).

[6] Enoki, T., Kobayashi, Y. and Fukui, K.I. (2007). Electronic structures of graphene edges and nanographene. International Reviews in Physical Chemistry, 26(4), 609-645.

[7] Wallace, P.R. (1947). The band theory of graphite. Phys. Rev., 71, 622-634.

[8] Ahmadi, M.T., Webb, J.F., Ismail, R., Rahmandoust, M. (2012). Carbon-Based Materials Concepts and Basic Physics, 65-98.

[9] Datta, S. (2005). Quantum Transport: Atom to Transistor, 2nd Edition, Cambridge University Press.

[10]Kargar, A. (2009). Analytical Modeling of Current in Graphene Nanoribbon Field Effect Transistors, 9th IEEE Conference on Nanotechnology (IEEE-NANO), 8, 710-712.

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