Int. J. Bio-Inorg. Hybr. Nanomater., 8(3): 119-124, Autumn 2019

Conductivity Coefficient Modeling in Degenerate and Non-Degenerate Modes on GNSs

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Received: 23 May 2019; Accepted: 27 July 2019

ABSTRACT: Carbon nanoscrolls (CNSs) with tubular structure similar to the open multiwall carbon nanotube have been of hot debate during recent years. Due to its unique property, Graphene Nanoscroll (GNS) have attracted many research groups' attention and have been used by them. They specially studied on energy storage devices such as batteries and super capacitors. These devices can be schematically assumed as rolled up graphene sheets with a spiral form. They are predicted to have high mechanical strength, high carrier mobility, and high thermal conductivity. 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. By utilizing a novel analytical approach, the current paper introduces modeling the conductance for graphene nanoscroll Furthermore, the conductance was modeled for both degenerate and non-degenerate regimes. Conductivity coefficient as a basic parameter in both degenerate and non-degenerate regimes was explored too.

Keywords: *Coefficient, Conductivity, Degenerate and non-degenerate regimes, Fermi-Dirac integral, Graphene Nanoscroll, Modes.*

INTRODUCTION

Graphene Nano-scrolls (GNS) is also one of the carbon-based materials that could roll the future by replacing silicon in common electronic applications such as computer, television, cell phone, and in most commonly silicon based technology. Many researches were carried out on the application of the Nano- scrolls, which is a very useful material, especially in energy storage devices such as batteries and super capacitors [1-3]. Unlike SWCNT, GNS is a spirally wrapped graphene sheet as shown Fig. 1. GNG is similar to the "Russian-Rolled" multiwall carbon nanotube (MWCNT), it is spirally wrapped from 2D graphene sheet into an ID tubular structure [4-6]. GNSs have attracted considerable attention as an open MWCNT-like tubular structure.

This carbon-based material can be schematically rolled up by a twisting of two-dimensional graphene sheets while it demonstrates a spiral form [7]. The spiral

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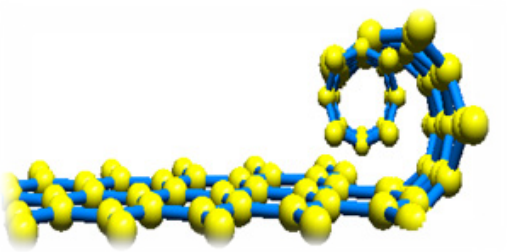

Fig. 1. Structural representations of GNS

wrapped GNS is expected to inherit excellent properties from both graphene and CNTs. Such properties can be achieved because of the individual topological structure, high mechanical strength, high carrier mobility, and high thermal conductivity of the GNC [8,9]. Due to the significant reduction of the Van-der Waals interactions between the inner and outer surfaces of graphene, the electronic band structure and phonon dispersion of GNS may differ from those of MWCNT and graphene nanoribbon, carbon-based materials. More researches, based on energy and hydrogen storage, were undergone because of their scroll topology with the variable intra-layer distance. For example, the flexible core with large surface area enables the GNSs to be applied for hydrogen storage and energy storage in super capacitors or batteries. The electrical-transport measurement of GNS indicates temperature dependence resistance [10,11]. Besides, GNS exists in the geometric forms of armchairs (n, n), zigzag (n, 0) and chiral (n, m). However, this material cannot be determined except with its chiral vector as single-walled nanotube (SWNT), whereby the small gap semiconductor or metallic for n-m is a multiple of 3. But for GNS, the energy gap oscillates significantly with the inner radius, thus changes its properties.

MATERIAL AND METHODS

Here, Nearest Neighbor Tight Binding (NNTB) energy model of graphene Nano-scroll presented is employed [12].

$$E = \pm t\left(1+4\cos\left(\frac{\sqrt{3}ka_{cc}}{2}\right)\cos\left(\frac{j\pi}{n}-\frac{\theta}{2n}\right)+\left(4\cos^2\left(\frac{j\pi}{n}-\frac{\theta}{2n}\right)\right)\right)^{\frac{1}{2}} \quad (1)$$

Where t is nearest neighbor C-C overlap energy which is normally between 2.5eV to 3.2eV. In the presented model, t=2.5 eV is used because of Chen's work and $a=\sqrt{3}a_{cc}$ is the length of basis vector or is known as Brava's lattice constant and k is the wave vector component around the circumferential direction which is quantized by the periodic boundary condition. Therefore, the derivation of the energy band structure and the density of states for GNS are very useful in gaining insights on its electrical properties. In addition, the other device physics parameter can be analyzed subsequence to this work. One of the unique capabilities of the GNS is to alter its electronic properties by changing its shape and diameter due to its open edges and no cap structure. The inter-planar distance can be diverse easily because it is open at both ends, which make the GNSs respond in a particular way towards doping or intercalation. The electronic and optical properties of the GNSs can be determined by performing the ab initio calculations based on density-functional theory and local density approximation to describe the ground state properties of the GNSs [13-15].

RESULT AND DISCUSSION

Based on the definition of conductance G=I/V, Boltzmann transport equation can be written as the Landauer Formula with,

$$G = \frac{2q^2}{h}\int_{-\infty}^{+\infty} M(E)T(E)\left(-\frac{df}{dE}\right)dE \quad (2)$$

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). Where M(E) is the number of modes which are above the cut-off at energy E in the transmission channel f(E) is Fermi-Dirac distribution function and T(E) is transmission probability. Note that in ballistic channel, T(E) is equal to one. Therefor the number of modes in the transmission channel can be:

$$M(E) = \frac{\Delta E}{l\Delta k} = \frac{\frac{6\hbar\sqrt{t}}{\sqrt{m^*}}\left(E-E_c\right)^{1/2}\Delta k}{l\Delta k} = \frac{\frac{6\hbar\sqrt{t}}{\sqrt{m^*}}\left(E-E_c\right)^{1/2}}{l} \quad (3)$$

Without scattering, electrons in ballistic transport behave according to the second law of Newton for motion of a particle at non-relativistic speeds. Thus, the electrical resistivity can be neglected in a ballistic channel of GNS due to the lack of scattering for electron transport. According to the number of sub-bands in equation (3) and Fermi–Dirac distribution function the conductance in equation (2), the conductance of GNS can be obtained by [16]:

$$G=\frac{2q^2}{h}\int_{-\infty}^{+\infty}\frac{6\hbar\sqrt{t}}{l\sqrt{m^*}}\left(E-E_c\right)^{1/2}\left(\frac{1}{K_BT}\right)\left(\frac{e^{\frac{E-E_f}{K_BT}}}{\left(1+e^{\frac{E-E_f}{K_BT}}\right)^2}\right)dE \quad (4)$$

Based on quantum confinement effect in GNS, conductance is a function of Fermi-Dirac integral, which is based on Maxwell approximation. Outside of the Dirac point, the conductance balances with the width of the GNS. Elastic scattering affects strongly the variation of total conductance fluctuations in graphene.

$$G=\frac{6q^2\sqrt{K_BTt}}{\pi l\sqrt{m^*}}\int_0^{\eta}x^{1/2}\frac{e^{x-\eta}}{\left(1+e^{x-\eta}\right)^2}dx \quad (5)$$

where $x=\frac{E-E_c}{K_BT},\eta=\frac{E_e-E_f}{K_BT},dE=K_BTdx$

By replacing $\eta\approx V_{GS}-V_T/k_BT/q$ in equation (5) the conductance relationship of GNS can be gained from equation below,

$$G=\frac{6q^2\sqrt{K_BTt}}{\pi l\sqrt{m^*}}\int_0^{\eta}x^{1/2}\frac{e^{x-\frac{q(V_{GS}-V_T)}{k_BT}}}{\left(1+e^{x-\frac{q(V_{GS}-V_T)}{k_BT}}\right)^2}dx \quad (6)$$

General mathematical model of GNSs conductance, which can be solved numerically, is presented by

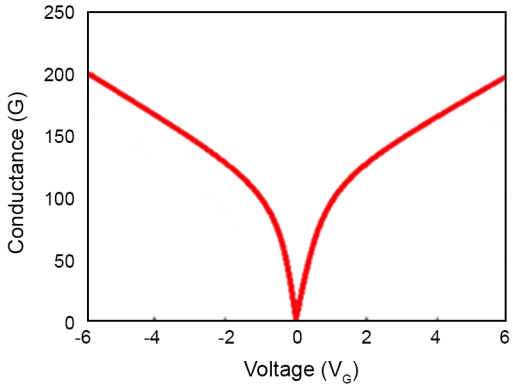

Fig. 2. Conductance model of GNS

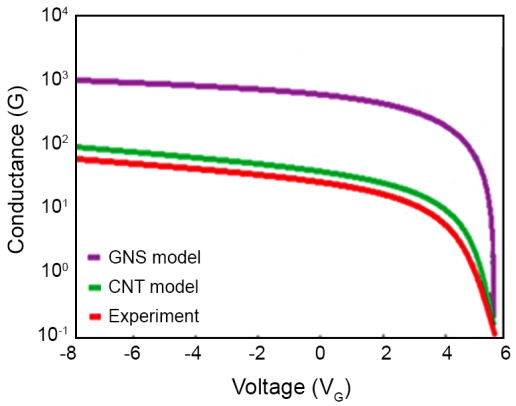

Fig. 3. G-V g characteristic of proposed the GNS model with experimental data for CNT

equation (6) where V_T is the biased thermal voltage and V_{GS} is the gate-source voltage. The analytical model of GNS conductance is plotted in Fig. 2.

In Fig. 3, the conductance of SWCNTs and GNSs is illustrated. By changing the gate voltage continually, the minimum conductance at the switch point where the density of electron and hole carriers is equal can be used to monitor the doping state of the SWCNT and GNS. This switch point also is known as the charge-neutrality point. As depicted in Fig. 3, in carbon nanotube surface, the conductance is dramatically decreased. As a result, it can be concluded that the conductance of the SWCNT and GNS channel would be very sensitive.

Therefore, in order to predict the GNS, the proposed model of the SWCNTs is carried out and compared with extracted experimental data for validation. In term of a semiconductor, in case the Fermi level is situated less than $3K_BT$ far away from the conduction and the valence band, or located within a band; degenerate approximation will play an important role on carrier statistics study. In the other words, in this regime $e^{x-\eta}$ in comparison with 1, can be neglected because the amount of x-η is very small. In the degenerate limit where Fermi Dirac distributions function has been approximated by f(E)=1. Therefore, the conductance for degenerate region can be written as [16];

$$G_d=\frac{2q^2}{h}\int_{-\infty}^{+\infty}\frac{6\hbar\sqrt{t}}{l\sqrt{m^*}}\left(E-E_c\right)^{1/2}\left(\frac{1}{K_BT}\right)\left(\frac{e^{\frac{E-E_f}{K_BT}}}{1+e^{\frac{E-E_f}{K_BT}}}\right)dE \quad (7)$$

Finally, the conductance model based on Fermi-Dirac

integral, can be written,

$$G_d = \frac{6q^2\sqrt{K_B Tt}}{\pi l\sqrt{m^*}}\int_0^{\eta} x^{1/2}\, e^{x-\eta}dx \qquad (8)$$

The conductance relationship can be gained from equation below,

$$G_d = \frac{6q^2\sqrt{K_B Tt}}{\pi l\sqrt{m^*}}\int_0^{\eta} x^{1/2}\left(\frac{e^{x-\frac{q(V_{GS}-V_T)}{k_B T}}}{1+e^{x-\frac{q(V_{GS}-V_T)}{k_B T}}}\right)dx \qquad (9)$$

Equation (9) can be analytically solved. Fig. 4 shows the general model of GNS conductance (red dots) and analytical solution in the degenerate approximation from equation (9). It is clear that the analytical degenerate approximation can be used instead of the general model out of the neutrality point. The conductance model of the SWCNT, the suggested model is closer to the experimental data; the conductance of the GNS/SWCNT dependent on the physical parameters such as diameter, length, radius and geometry of the GNS and SWCNT channel. The result of this comparison between the SWCNT and GNS conductance models indicates that the GNS shows a superior conductance. Structural parameters of the GNS are somewhat different from the SWCNT, but the things that remain the same are the certain factors in affecting their electronic properties. Each of these materials has its own structural parameter that influences the electrical properties, though some of the GNS behavior can be related to the SWCNT by its diameter. The electronic properties of SWCNTs are very much influenced by the size of their diameter. However, the electronic properties of GNSs are related to the number of overlapping layers, which can be referred to as N turn.

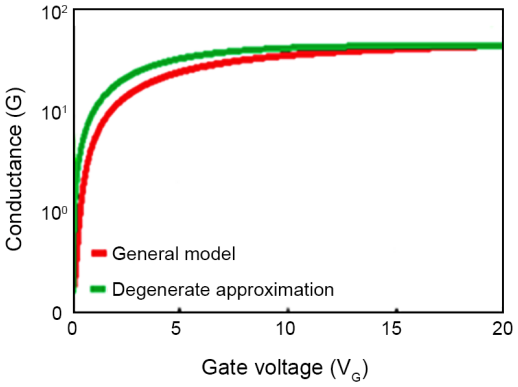

Fig. 4. General model of GNS conductance (red dots) and Analytical solution of the degenerate approximation (green dots).

In the non-degenerate regime, the Boltzmann approximation can be used, $f(E)=\exp(E_f-E/K_B T)$. The conductance in non-degenerate regime can be modified by exponential function so that;

$$G_{nd} = \frac{2q^2}{h}\int_{-\infty}^{+\infty}\frac{6\hbar\sqrt{t}}{l\sqrt{m^*}}\left(E-E_c\right)^{1/2}\left(\frac{e^{\frac{E-E_f}{K_B T}}}{K_B T}\right)\left(e^{\frac{E_f-E}{K_B T}}\right)^2 dE \qquad (10)$$

The conductance model based on Fermi-Dirac integral, can be written,

$$G_{nd} = \frac{6q^2\sqrt{K_B Tt}}{\pi l\sqrt{m^*}}\int_0^{\eta} x^{1/2}\, e^{-(x+\eta)}dx \qquad (11)$$

The conductance against gate voltage for the general state and both degenerate and non-degenerate regimes are plotted in Fig. 5 indicating that for the degenerate regime, it has been less than influenced by η variations. The calculation shows that the non-degenerate approximation can be used instead of the general model in neutrality point. Fig. 5 shows GNS conductance model in the non-degenerate regime based on equation (11). Green dots are the non-degenerate approximation and red dots are general model. In non-degenerate regime, the normalized Fermi level, to decrease by increasing the temperature. It is actually shown that by altering gate voltage through the GNS controlling elements, the G–Vg characteristic curve can be managed. Also, the results compared with experimental data and there is good agreement between results and experimental data.

GNSs working based on quantum current, the dia-

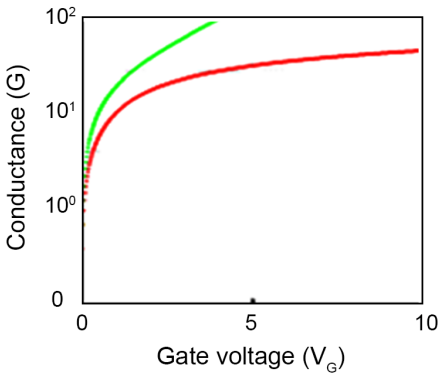

Fig. 5. The non-degenerate approximation (green dots) and general model of GNS conductance (red dots).

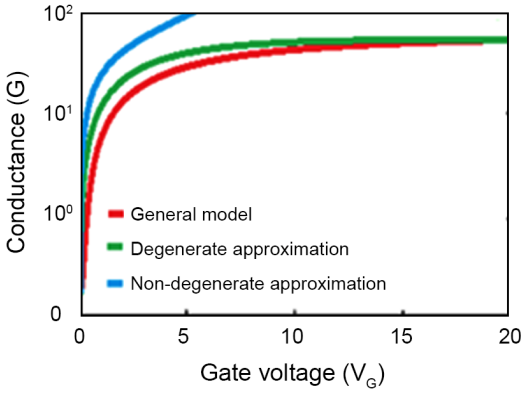

Fig. 6. The general model (red dots), degenerate approximation (green dots) and non-degenerate approximation of GNS conductance (blue dots).

gram current-voltage and conductance is too close to degenerate states. In Fig. 6, general model, degenerate approximation and non-degenerate approximation for GNS show. Our method indicates that near the neutrality point, the non-degenerate approximation can be used properly showing the temperature dependence relation in conductance as well. In contrast, out of this boundary condition it is estimated to work in the degenerate regime. Moreover, it confirms that GNS conductance is temperature dependent near the neutrality point as reported in experiments. Minimum conductance is depended on temperature and increases by increasing temperature near the neutrality point but beyond the neutrality point conductance is independent of temperature. The results obtained from the proposed model agree with the published experimental data.

CONCLUSION

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. Graphene Nano-scrolls (GNSs) with one-dimensional band energy which leads to unique electrical properties such as high mechanical strength, high carrier mobility, and high thermal conductivity have been discussed. The study focused on GNS and analytical model of Conductivity coefficient that was initially presented. Conductivity coefficient as a basic parameter in both degenerate and non-degenerate regimes was explored too. 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 conductivity coefficient for graphene Nano-scroll Furthermore. Finally, comparison with experimental data will show the validity of the GNS model. In GNSs, Minimum conductance is depended on temperature and increases by increasing temperature near the neutrality point but beyond the neutrality point conductance is independent of temperature. The results obtained from the proposed model agree with the published experimental data.

ACKNOELDGMENTS

Authors would like to acknowledge the financial support from Research University grant of the Urmia University. Also thanks to the Re¬search Management Center of Urmia University for providing excel¬lent research environment in which to complete this work.

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