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QUANTUM CURRENT MODELLING ON GRAPHENE NANOSCROLLS

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ABSTRACT: - Graphene has amazing carrier transport property and high sensitivity at the single molecule level which leads them as a promising material for biosensor application. In order to develop the new device types same as graphene nanoribbon, Carbon Nanotube Field Effect Transistor (CNTFET) and Nanowire, it is essential to investigate of quantum limit in low dimensional devices. In this paper quantum current of Monolayer Graphene Nanoscroll (MGNS) is modelled and the electronic properties due to the dependence on structural parameter are analyzed. In addition 1D quantum transport coefficient based on the approximation of the wave vector relation for MGNS is presented.

Keywords: quantum transmission, quantum current, degenerate limit, non-degenerate approximation, Graphene Nanoscroll.

1. INTRODUCTION

Graphene Nanoscroll (GNS) with spiral structure have been considered as rolled up Graphene with one dimensional structure as shown in figure (1)[1, 2]. The wet chemistry technique as a simple fabrication method on GNS production have been suggested[3-5] also by hydrogenation on one side it can be scroll up into a graphene nanoscroll (GNS) completely which is stable at room temperature[6, 7].In addition based on the Raman characteristics of nanoscrolls the new bands ,G-peak and D-peak in the low-wave number region have been measured [8]. Also GNS transport properties in the presence of uniform electric field has been investigated [9].Graphene nanoscrolls because of unique electronic and physical properties such

as high carrier mobility, unconventional quantum Hall effect together with potential applications in nanoelectronics make them attractive research platforms [10-15]. Also their possible application on high speed switching devices has been concerned [14]. In addition the tuneable band gap on graphene nanoscrolls(GNS) lead to the field-effect transistors (FET) application as shown in figure 2 [16-19].

The theoretical description on electron transport in a bridge system of GNS has been completed and the fundamental mechanisms underlying the electron transport in bridge systems have been addressed. In addition experimental data on electron transport indicates disagreement between the theory and experiment. There are some controlling parameters such as the geometry of the conducting channel between the two electrodes, the coupling of the bridging material, the current amplitude, the quantum interference effect. Moreover, the dynamical instability in the nano-scale devices can control the electron transport as well. However, a little information has been published about the role of quantum effects in GNS MOSFET. In this paper, quantum transmission on GNS is presented and also the current-voltage characteristic based on quantum transport phenomenon is modelled. The electronic properties due to the structural parameters are analyzed. In addition 1D quantum transport based on the wave vector approximation on GNS is presented.

2. MODEL

Electrons in the presence of potential discontinuity will face non zero probability of reflection and transmission. Classically the transmission in the junction is occurred when the initial energy of electron is extra than the potential discontinuity. On the other hand based on the tunnelling effect there is non-zero probability of transmission in the junctions. Therefore by considering a channel region in the transistor in the form of barrier as shown in figure 3 the transmission coefficient is calculated and respected current is plotted.

There are three regions associated with the proposed structure and wave function on first region is assumed[20] as:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 = E\psi_1 \Rightarrow \psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \qquad (1)$$

In the second region there is a discontinuity in the potential and the Schrodinger equation is modified in the form of:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V(x)\right)\psi_2 = E\psi_2 \Rightarrow \psi_2 = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \qquad (2)$$

As the left side material is assumed to be similar to the right side but the wave form in the right hand is travelling wave and in the left hand is standing wave therefore the wave function is written as[9]:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_3 = E\psi_3 \Rightarrow \psi_3 = A_3 e^{ik_3 x} \qquad (3) \qquad \text{where } k_1 = k_2$$

As shown in figure 3 the boundary condition is summarized as

$$\begin{aligned} &\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi'_1(0) = \psi'_2(0) \\ &\psi_2(a) = \psi_3(a) \quad \text{and} \quad \psi'_3(a) = \psi'_2(a) \end{aligned} \qquad (4)$$

These boundary conditions are applied to get the transmission coefficient with respect to the quantum transmission coefficient definition. The quantum transmission coefficient indicates number of electrons can overcome to the junction barriers in the channel. The general definition for quantum transmission coefficient is given by[21]

$$T = \left|\frac{A_3}{A_1}\right| = \frac{4\left(\frac{2m}{\hbar}\frac{2E}{3ta_{cc}}\right)\left(\left(E-E_g\right)\right)}{4\left(\frac{2mE}{\hbar}\right)\left(\left(E-E_g\right)\frac{2}{3ta_{cc}}\right)+\left(\left(\frac{2mE}{\hbar}\right)+\left(\left(E-E_g\right)\frac{2}{3ta_{cc}}\right)\right)^2 Sinh^2\left(\left(\left(E-E_g\right)\frac{2}{3ta_{cc}}\right)^{1/2} L\right)} \qquad (5)$$

For the first and last regions in the parabolic band energy limits, the wave vector can be assumed in the form of $k_1 = k_3 = \left(\frac{2mE}{\hbar}\right)^{1/2}$. However because of possible band gapformation in the GNS the quantum wave vector in the second region is calculated as:

$$\left(\left(E - E_g\right)\frac{2}{3ta_{cc}}\right)^{1/2} = k_2 \qquad (6)$$

Where $E_g = \frac{3ta_{cc}b^2}{4}$ is the band gap energy and $b=\left(\frac{2\pi}{a_{cc}\sqrt{3n}}\right)\left(\nu-\left[\frac{2n}{3}+\frac{\varphi}{2\pi}\right]\right)$. Quantum current based on the Landauer formalism have been reported [22, 23] as:

$$I_d=\int_0^{\eta}F(E)T(E)dE=\frac{AK_BTx\left(K_BTx+E_g\right)}{AK_BTx\left(K_BTx+E_g\right)+\left(B\left(K_BTx+E_g\right)+CAK_BTx\right)^2 Sinh^2\left(CL^2AK_BTx\right)^{1/2}}\frac{dE}{e^{x-\eta}+1} \qquad (7)$$

Where $A=\left(\frac{16m}{3\hbar ta_{cc}}\right)B=\left(\frac{2m}{\hbar}\right)C=\frac{2}{3ta_{cc}}$, F (E) is Fermi Dirac distribution function which illustrates the probability of occupied levels at energy E and that can write as:

$$f(E)=\frac{1}{\exp\left(\frac{E-E_F}{k_BT}\right)+1} \qquad (8)$$

In the simplified form by considering the wave vector and quantum transmission coefficient the quantum current is modified as

$$I=\int_0^{\eta}\frac{AK_BTx\left(K_BTx+E_g\right)}{AK_BTx\left(K_BTx+E_g\right)+\left(B\left(K_BTx+E_g\right)+CAK_BTx\right)^2\left(CL^2AK_BTx+\frac{\left(CL^2AK_BTx\right)^2}{3}\right)}\frac{dE}{e^{x-\eta}+1}$$

By increasing the number of carriers, device will operate in degenerate limit. Degenerate regime plies an important role on quantum current study in the nano-scale devices. In the degenerate regime, $E-E_F<3k_{BT}$, also, degeneracy on GNS can be defined by the Fermi probability equal to one ($f(E)=1$). In the contrary for the non-degenerate regime, $E-E_F>3k_{BT}$, the Boltzmann approximation can be used,

$$f(E)=\exp\left(\frac{E_F-E}{k_{BT}}\right) \qquad (10)$$

Which means in the conduction band the concentration of electrons pass the density of states, the Fermi energy lies in the conduction band[24]. In the other words, because of the very small amount of x-η in this regime, exp (x-η) can be neglected. So for quantum current in degenerate approximation we can write

$$I_d=\int_0^{\eta}\frac{4c_1c_2\left(x+d\right)xK_BTdx}{4c_1c_2\left(x+d\right)x+\left[\frac{c_2^3L^3x^3}{6}+c_2Lx\right]^2\left(c_1\left(x+d\right)+c_2x\right)^2} \qquad (11)$$

Non-degenerate approximation have been shown with the distance more than $3K_BT$ from either the conduction or valance band edge in the form of band gap near the Fermi level. As shown in figure (4) in semiconductors, non-degenerate regime is located in a band with distance less than $3K_BT$ far away from the conductance and the valence band therefore the normalized Fermi energy less than -3indicates non-degenerate approximation. Hence, Fermi integral in non-degenerate regime can be modified by exponential function as:

$$I_{nd}=\int_0^{\eta}\frac{4c_1c_2\left(x+d\right)xK_BTe^{\eta}dx}{4c_1c_2\left(x+d\right)x+\left[\frac{c_2^3L^3x^3}{6}+c_2Lx\right]^2\left(c_1\left(x+d\right)+c_2x\right)^2} \qquad (12)$$

Based on the presented model quantum current as a basic characteristic of a transistor is simulated and compare to the conventional methods same trend is recognized.

3. CONCLUSION

Graphenenanoscroll has amazing carrier transport property and high sensitivity at the si ngl molecule level which leads them as promising materials in biosensor application. In order to develop the new device types same as graphene nanoribbon , Carbon Nanotube Field Effect Transistor (CNTFET) and Naonowire it is essential to investigate the quantum limit in low dimensional devices. In this paper quantum current of Monolayer Graphene nanoscroll (MGNS) is modeled and the electronic properties due to the structural parameter is analyzed. In addition 1D quantum transport coefficient based on the approximation of the wave vector relation for MGNS is presented.

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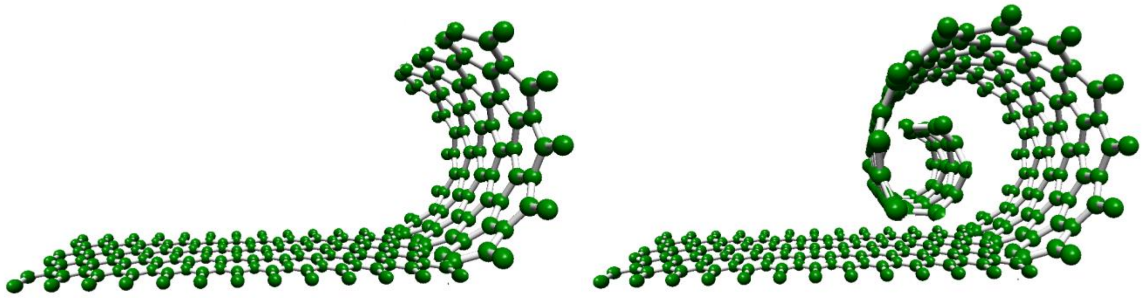


Figure (1): Graphene Nanoscroll geometries

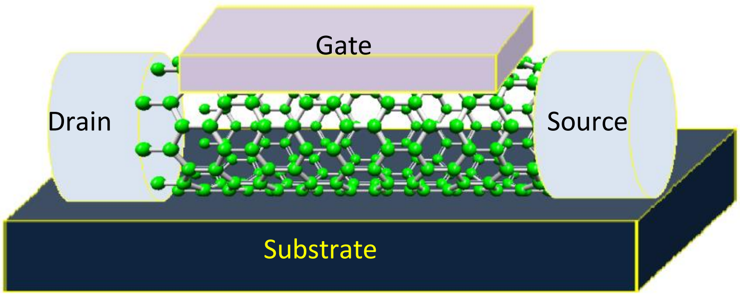
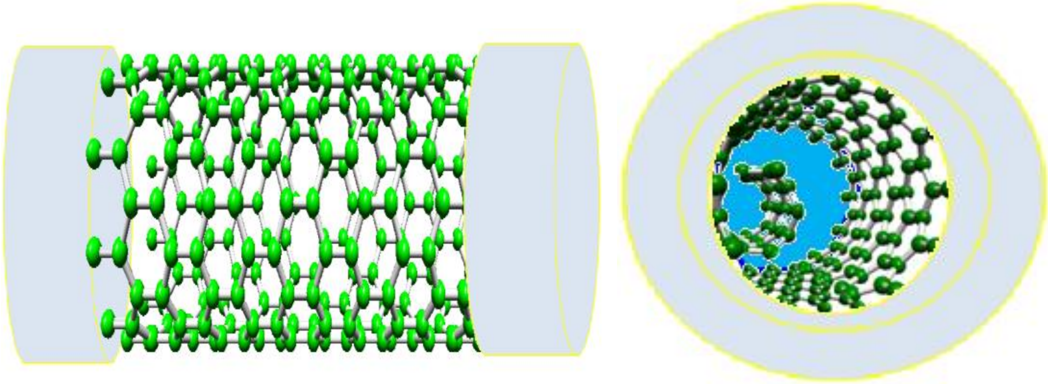


Figure (2): Armchair and zigzag geometries



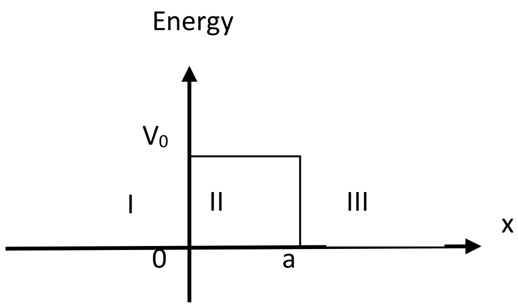


Figure (3): Channel region barrier in GNS MOSFET

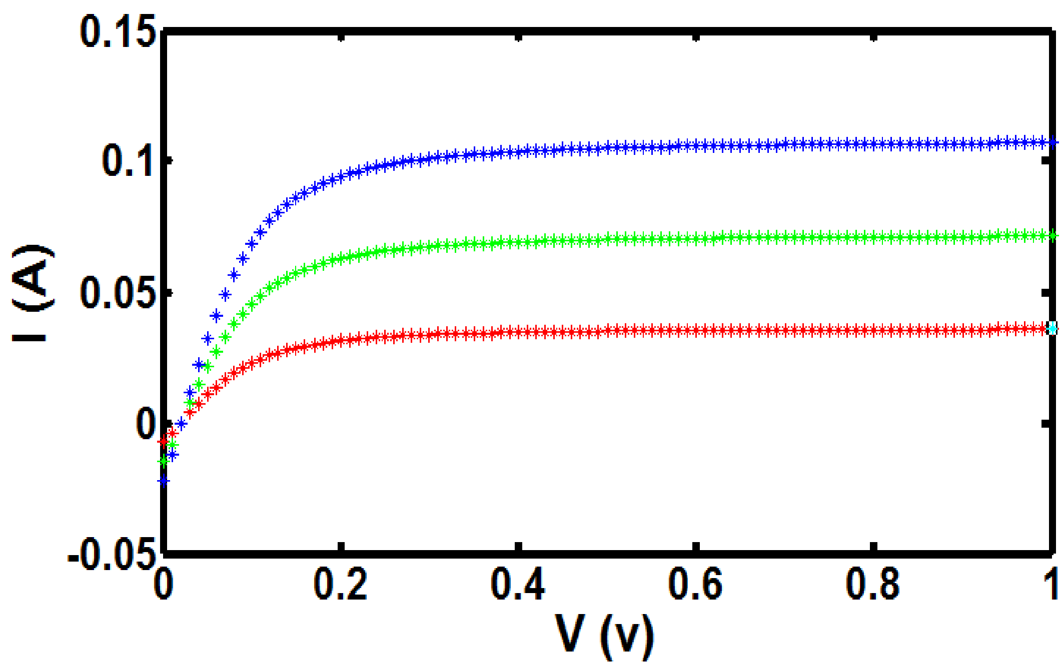


Figure (4): the I-V characteristic in GNS MOSFET

نمذجة التيار الكمي في جرافين نانوسكورلس

ملخص البحث

الجرافين يمتلك خاصية عالية في نقل الناقل وتحسس عالي في مستوى جزيءالواحد مما يجعلها مادة واعدة لتطبيق في جهاز الاستشعار البيولوجي. من اجل تطوير انواع من الاجهزة الحديثة تشابه (graphene nanoribbon, Carbon Nanotube Field Effect Transistor (CNTFET) and Nanowire) و تعتبر من اجهزة الابعاد. في هذا البحث التيار الكمي في جرافين نانوسكورل احادي الطبقة هو نمذجة و الخصائص الالكترونية بسبب الاعتماد على ضرورة التحقق من الحد الكمي في ادنى اجزاء بنيوي ليتم تحليله. بالأضافة الى ذلك , معامل النقل الكمي ذات البعد الواحد تستند على تقريب علاقة ناقلات موجة لجرافين نانوسكورل احادي الطبقة المعطى.