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Quantum current modeling in nano-transistors with a quantum dot

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ABSTRACT: Carbon quantum dots (CQDs) serve as a new class of 'zero dimensional' nanomaterial's in the carbon class with sizes below 10 nm. As light emitting nanocrystals, QDs are assembled from semiconductor materials, from the elements in the periodic groups of II-VI, III-V or IV-VI, mainly thanks to impacts of quantum confinement QDs have unique optical properties such as brighter, highly photo and chemical stable, with broad absorption, narrow and symmetric emission spectrum. A substantial QDs feature is that their emission wavelength can be fine-tuned by adjusting their size and chemical composition. Nowadays carbon nanoparticles are applied on the island of single electron transistor and Nano-transistors, and fluorine because its sustainability is one of the best materials inter alia. The basis of Single electron devices (SEDs) is controllable single electron transfer between small conducting "islands". In this paper transmission coefficient as a main transport factor need to be explored in this work the transmission coefficient and reflection coefficient for a potential barrier is investigated. All theoretical expressions such as height, width of potential barriers, distance between them and carrier property are included to have exact value of transmission coefficient. Then quantum current of double barrier single electron transistor (SET) is modeled and models current-voltage characteristic based on quantum transport and the electronic properties due to the dependence on structural parameter are analyzed.

Keywords:*Barrier; Quantum Current; Fullerene; Island;Single Electron Transistor.*

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INTRODUCTION

Carbon quantum dots (CQDs) serve as a new class of 'zero dimensional' nanomaterial's in the carbon class with sizes below 10 nm. They were initially discovered during modification of single-walled carbon through preparative electrophoresis in 2004 and laser ablation of graphitic powder and cement in 2006. As light emitting nanocrystals, QDs are assembled from semiconductor materials, from the elements in the periodic groups of II-VI, III-V or IV-VI, mainly thanks to impacts of quantum confinement QDs have unique optical properties such as brighter, highly photo and chemical stable, with broad absorption, narrow and symmetric emission spectrum. A substantial QDs feature is that their emission wavelength can be fine-tuned by adjusting their size and chemical composition. The known names for zero-dimensional structure called nanoparticles, clusters, colloids, nanocrystals, and fullerenes. They are ranged various tens to a few thousand atoms in scale. In all three directions electrons are contained. The most famous zero-dimensional structure is Bucky ball.

In September 1985, fullerenes were discovered in an experiment for the first time. Other fullerenes were discovered immediately with more and less carbon atoms; it is worthy to note they were ranged from 18 atoms to up to hundreds of atoms. Among them, the Bucky ball with 60 carbon atoms is the most obvious. C_{60} is the easiest product and the cheapest material, whose prices is rising rapidly for other bigger fullerenes. They might be found in three various forms: spherical, elliptical and tubes. The C_{60} Bucky ball structure is an integration of 12 pentagonal and 20 hexagonal rings, in turn creates a spheroid shape with 60 vertices for 60 carbons. Fig. 1 illustrates structure of the molecule, showing ways of pentagonal rings location at the vertices of an icosahedron so that none of two pentagonal rings are settled next to each other. The mean C-C bond distance calculated by nuclear magnetic resonance (NMR) is found to be 1.44 A°. A diameter of 7.09 A° is calculated for the C_{60} as C-C distance is equal to 1.40 A° for the hexagon bonds and 1.46 A° for the pentagonal bonds length (Li, *et al.,* 2012). As the third form of carbon fullerenes, have been converted to important molecules in science and technology application (Welsher, *et al.,* 2009). Because of their very practical characterizes, fullerenes serve as a key topic on nanotechnology and industrial research todays (Anton, *et al.,* 1996). At the same time fullerenes are applied in today's industry, especially in cosmetics, in which they have great contributions as antioxidants (Eulises Ulloa, 2013).

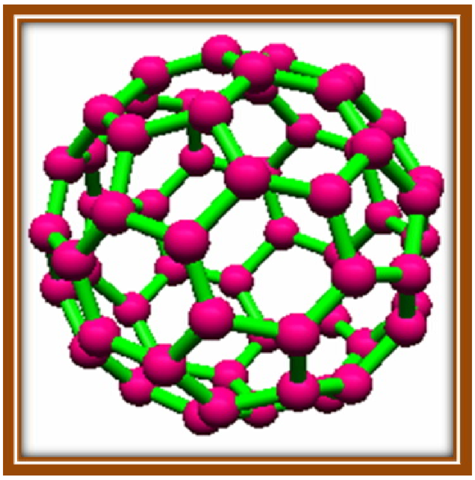

Fig. 1. C_{60} Molecular Structure

Having less than 100 nm in diameter Quantum dot is a mesoscopic system where electrostatic energy or coulomb energy can be changed due to single electron removal or addition which greater than the thermal energy and may control electron transfer into and out of the quantum dot.

In other words, having a tunable number of electrons occupying discrete orbitals Quantum dot is a small conducting island. As it can be seen in Fig. 2, a tunnel junction is served as a thin insulating barrier among two conducting electrodes.

No current can flow through an insulating barrier as for classical electrodynamics. But there is some probability (i.e. greater than zero) for an electron located at one side of the barrier (tunnel junction) to reach the other side as per the quantum mechanics method. Hence, the transfer of electrons through the barriers between the quantum dots would lead to charging neighboring quantum dots.

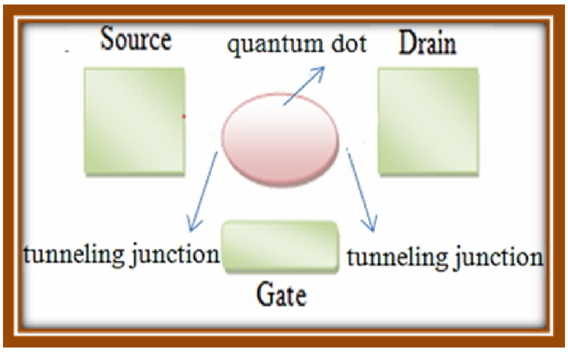

Fig. 2. Schematic structure of SET showing tunnel junctions.

In case, an electron tunnels through the barrier (tunnel junction) into the quantum dot once the voltage V exceeds Vt. Single electron circuits with Single Island and with multiple island are shown in Figs. 3and 4.

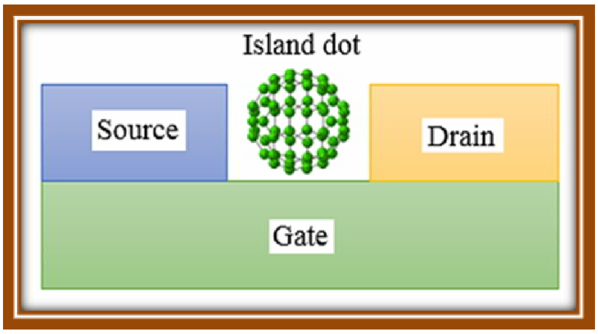

Fig. 3. Single electron transistor circuits with Single Island.

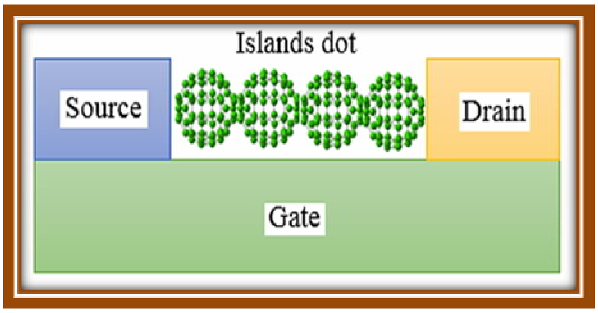

Fig. 4. Single electron transistor circuits with multiple islands.

To conceptualize coulomb blockade of tunneling more exactly, we again consider the single electron circuits in which on applying bias voltage in which a current flow can be found. Now, the first order approximation tunneling current is proportional to the applied bias voltage if we prevent additional effects, on the other side, it can be noted that a tunnel junction behaves as a resistor having constant value contingent upon barrier thickness. Since, the tunnel junction is consisted of two conductors and an insulating layer between these two conductors. Hence, tunnel junction can be defined by the tunnel resistance R and tunnel capacitance C. Now, under such circumstance, if the bias voltage is lower than the voltage developed in the tunnel junction the electric current is suppressed. Furthermore, a gradual increase in tunnel junction resistance around zero bias is served as the coulomb blockade. So, coulomb blockade may be defined as the increased tunnel junction resistance at very low bias voltages of an electronic device in turn consists of at least one low capacitance tunnel junction.

MATERIAL AND METHODS

In quantum mechanics, the values of the bands with potential barriers one dimensional are scattered.Based on the important points in quantum mechanics, when a wave passes through several spatial regions with different boundaries, the wave function of the first region differs from the second and third wave functions. But the boundary conditions are similar in neighboring areas. So the single electron transistor is divided into three sections, Source, Drain, and Island,(Gupta, 2016) that in Fig. 5 energy as a function of the length of a single-electron transistor channel with a potential barrier is plotted.In this research, used islands of carbon nanoparticles and the ability of the carbon material in addressing these constraints is checked.

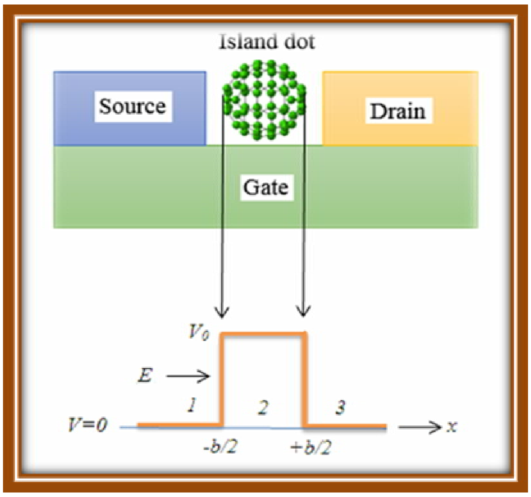

Fig. 5. A barrier channel region in single electron transistor.

Then, the current of the transistor is modeled on Florin Island. The transmission coefficient once the wave propagating in a medium with discontinuities is considered as:

$$T = \left| \frac{j_{transmitted}}{j_{incident}} \right| = \left| \frac{A_{n+1}}{A_n} \right|^2 \quad (1)$$

This equation is rewritten in the presence the wave vector therefore the spin per valley in carbon nanoparticles can be modified as:

$$T = \frac{1}{1 + \left(\frac{k_1^2 + k_2^2}{2k_1 k_2} \right)^2 Sinh^2(k_2 L)} \quad (2)$$

The transistor operation can be modeled in the form of three different regions as shown in Fig. 5 which leads to the Schrödinger equation result for potential of each region as;

$$V(x)=\begin{cases}0 & , \quad x\langle\frac{-b}{2}\\ V_0 & , \quad \frac{-b}{2}\langle x\langle\frac{b}{2}\\ 0 & , \quad x\rangle\frac{b}{2}\end{cases}\Rightarrow \psi(x)=\begin{cases}A_n e^{ikx}+B_n e^{-ikx} & , \quad x\langle\frac{-b}{2}\\ Ce^{-Kx}+De^{Kx} & , \quad \frac{-b}{2}\langle x\langle\frac{b}{2}\\ A_{n+1}e^{ikx}+B_{n+1}e^{-ikx} & , \quad x\rangle\frac{b}{2}\end{cases} \quad (3)$$

Where wave number in first and third regions is $k=\sqrt{\frac{2mE}{\hbar^2}}$, and the wave number in channel region is $K=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$, As the transmission for E<V_0. The absolute square of which give the transmission probabilities T. These are:

$$\mathrm{T}=\frac{4\mathrm{k}^2\mathrm{K}^2}{-\mathrm{k}^4+2\mathrm{k}^2\mathrm{K}^2-\mathrm{K}^4+\left(\mathrm{k}^4+2\mathrm{k}^2\mathrm{K}^2+\mathrm{K}^4\right)\cosh^2(\mathrm{bK})} \quad (4)$$

We can plot the transmission probability against the energy of the incident beam of particles. It is discovered that the performance of the transmission $T(E)$ is increased rapidly while the energy of the electron is less than the barrier height energy (E<V_0) on the other hand for the energies more than the potential barrier the transmission is saturated at 1 as expected. But the presented model needs to be modified for this region to get the accurate results. In the presence of k^2 and K^2 the transmission can be modified as:

$$T(E)=\frac{4\alpha}{-1+2\alpha-\alpha^2+(1+2\alpha+\alpha^2)\cosh^2(\beta\sqrt{\frac{\alpha}{1+\alpha}V_0 b})} \quad (5)$$

We define;

$$E=\frac{V_0}{1+\alpha},\beta=\sqrt{\frac{2m}{\hbar^2}},x=\frac{E-E_g}{k_BT},\eta=-\frac{E_g-E_f}{k_BT}$$

RESULT AND DISCUSSION

On the other hand based on the Landauer formalism quantum current have been reported as:

$$I=\int_{E-\frac{E_g}{2}}^{E+\frac{E_g}{2}} T(E)f(E)dE \quad (6)$$

Where F(E) is Fermi-Dirac distribution function which implies the probability of occupied levels at energy E. It has been reported that the quantum current in the minimum uncertainty overlaps with the classical current (Anderson, *et al.,* 2009, Yano, *et al.,* 1994).

Additionally nanoscale devices because of quantum confinement effect operates in quantum limit therefore the quantum current as a general form of current is considered. Based on the proposed structure and reported quantum coefficient the quantum current is modified as:

$$I=\int_0^{\eta}\frac{4\alpha K_BT}{-1+2\alpha-\alpha^2+(1+2\alpha+\alpha^2)\cosh^2(\beta\sqrt{\frac{\alpha}{1+\alpha}}V_0b)}*\frac{1}{1+e^{x-\eta}}dx$$

(7)

This equation is numerically solved for different applied voltages. Thus, the proposed quantum current model illustrate acceptable trends by graphene nanoribbon based schottky transistor and its I-V characteristic as a main transistor characteristic is presented in Fig. 6.

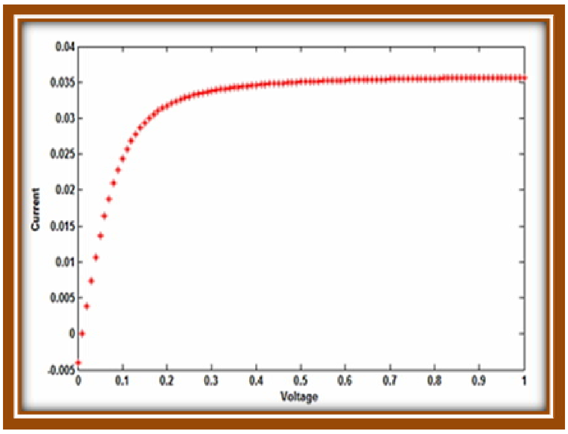

Fig. 6. I-V Characteristic based on the presented model for single electron transistor.

The transistor operation on degeneracy limit as an important working schemes need to be explored. As the number of carrier's increases, device goes to the operation mode in degenerate limit which plays an important role on the nano-scale device modelling (Hedayat, *et al.*, 2016). The degenerate regime $(E-E_F<3k_BT)$ can be defined in the form of probability function as well, once the Fermi probability function equals to one, $(f(E)=1)$ on the contrary for the non-degenerate regime, $(E-E_F>3k_BT)$ then we can write $f(E)=\exp\left(\frac{E_F-E}{k_BT}\right)$ (Hedayat, *et al.*, 2016),shown in Fig. 7 in the conduction band, where concentration of electrons pass the density states, the fermi energy lies in the conduction band.

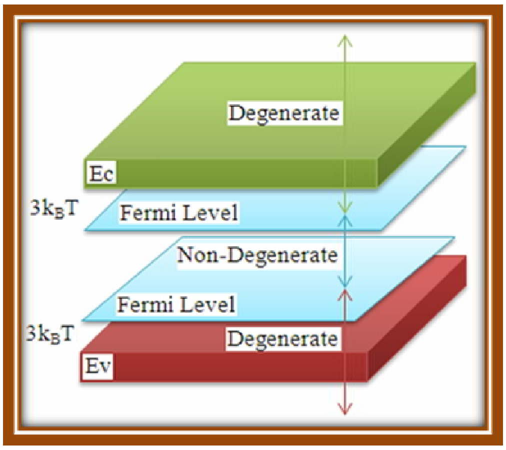

Fig. 7. Comparison of the degenerate regime and non-degenerate regimes.

In the other words the amount of x-η is very small in this regime therefore the expo(x-η) can be neglected in comparison by one so the quantum current in degenerate approximation is:

$$I_d=\int_0^{\eta}\frac{4\alpha x K_BT}{-1+2\alpha-\alpha^2+(1+2\alpha+\alpha^2)\cosh^2(\beta\sqrt{\frac{\alpha}{1+\alpha}}V_0b)}dx$$

(8)

As depicted in the Fig. 8, quantum current in the range larger as zero leads to the degenerate approximation in carbon nanoparticles.

On the other hand the non-degenerate approximation appears when the distance increases more $3K_BT$ in energy from either the conduction or valance band edge in the form of band gap near the Fermi level.

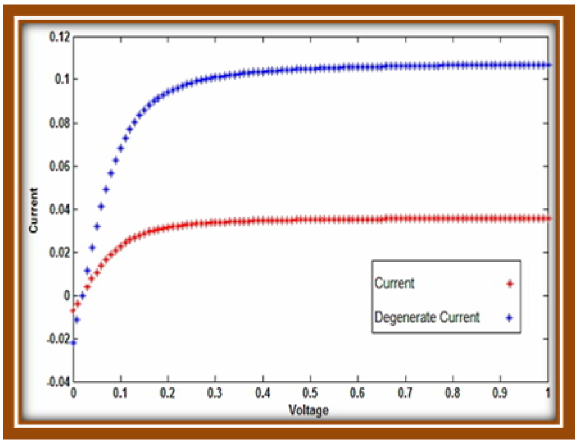

Fig. 8. I-V Model of graphene Nano ribbon in degenerate approximation.

In semiconductors, non-degenerate region is nestled in a band with distance less than $3K_BT$ beyond the conduction and valence band. Hence, the current in non-degenerate regime can be modified by exponential function:

$$I_{nd} = \int_0^{\eta} \frac{4\alpha x K_B T e^{\eta}}{-1+2\alpha-\alpha^2+(1+2\alpha+\alpha^2)\cosh^2(\beta\sqrt{\frac{\alpha}{1+\alpha}}V_0 b)} dx \quad (9)$$

As shown in Fig. 9 it is concluded that quantum current on degenerate regime provides high quantum current compare to the non-degenerate limit. Based on the proposed model the quantum current is simulated numerically as a basic characteristic of a transistor and similar to the conventional systems Ohmic and saturation regions are recognized.

CONCLUSIONS

The single-electron transistors are a fast-moving component in the nanoscale, which switches the

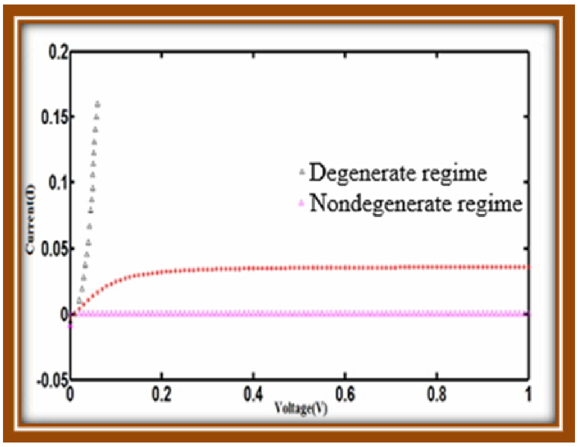

Fig. 9. Comparison of the quantum current(I) in degenerate(I_d) and non-degenerate limits (I_{nd}).

current through electron tunneling between the coulomb barriers.Thus, fullerene with high electron mobility is selected as the structural material of a single electron transistor withislands. By adjusting the length of the island and the voltage applied to the gate the current can be obtained with the desired value. In this paper quantum current of double barrier single electron transistor (SET) is modeled and models current-voltage characteristic based on quantum transport and the electronic properties due to the dependence on structural parameter are analyzed.

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