J. Basic. Appl. Sci. Res., 2(10)10783-10787, 2012

ISSN 2090-4304
Journal of Basic and Applied Scientific Research
www.textroad.com

Transport Properties of Graphene Nanoribbon Quantum Dots in The Presence of Disorder

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ABSTRACT

The electronic transport properties of a graphene nanoribbons quantum dot (GNRQD) are investigated by means of the Landauer approach using tight-binding model. We find that the transmission coefficient of the electrons decreases in the presence of random disorder. The presence of the random disorder causes the wave function to be localized. In this manner, we emphasize that when the disorder density is sufficiently high, the transmission coefficients and the current reduces due to multi-scattering phenomenon. Furthermore from the *I-V* curve we found the "current quantization" in the system. These theoretical results can be considered as a base for development in designing graphene nanodevices.
KEYWORDS: electronic transport; graphene nanoribbons quantum dot; Landauer; disorder.

1. INTRODUCTION

In the last eight years, graphene has attracted much attention from the scientific community for its interesting fundamental properties, most of them resulting from the massless Dirac fermion nature of the electrons in such a material, and for its potential applications, including the development of highly integrated microelectronics [1]. The unusual transport properties of graphene arise from its linear E-K relation from low energies near the six corners of two-dimensional hexagonal Brillouin zone [2]. However, as all the other materials, real graphene device also includes some disorder. Unlike carbon nanotubes, graphene ribbons have edges that are vulnerable to disorder that could limit the localization length, and hence, the length over which ballistic transport could occur [3]. Disorder effects in graphene are of particular importance on the account of its two dimensional (2D) lattice structure [4]. The single-parameter scaling theory predicts that in 2D systems, arbitrary weak disorder leads to Anderson localization of the single-particle wave function [5].For graphene nanoribon, Shi-Jie et al. investigated the Anderson localization of fermions at the Dirac point with different type of disorder and found that in the case disorder all states are localized as predicted by the scaling theory for two-dimensional [6]. Indeed, localized states in disordered graphene near Dirac points have been observed experimentally and numerically [7], [8]. In the following, we analyze the effects of disorder in graphene nanoribbons quantum dots (GNRQDs).The disorder (Anderson-type) is introduced via random fluctuations of the on-site energies of the π orbitals, which mimic a short range scattering potential that has been widely studied in the past as a generic disorder model in the framework of localization theory[9]. In addition, quantum dot can be realized regardless of substrate induced static disorder or irregular edges of the junction. This device can be used to easily design quantum dot devices. This platform can also be used to design zero-dimensional functional nanoscale electronic devices using graphene ribbons.

2. MODELLING

The GNRQD is shown in Fig. 1. The systems could be divided into three regions, left, right and the region between them, namely device. The tight - binding Hamiltonian of the GNRQD can be written as: [11]

$$H = \sum_i \varepsilon_i a_i^+ a_i + t \sum_{i,j} e^{i\varphi_{ij}} a_i^+ a_j + \sum_i V a_i^+ a_i \qquad (1)$$

The low energy electronic properties of 2D graphene are accurately described by the π-orbital tight-binding Hamiltonian, which is a first nearest neighbor two centers orthogonal *pz* model, with on-site energies $\varepsilon_0 = 0ev$ for all orbitals and the hopping term $t = 2.7ev$. To mimic short range disorder, Anderson type disorder is introduced as a random fluctuation of the on-site energies of the Hamiltonian $(\varepsilon_i = \varepsilon_0 + \delta\varepsilon)$. The scattering potential can thus be characterized by a single parameter w which defines the range of energy variations $\delta\varepsilon \in [-wt/2, wt/2]$,and thus

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allows us to tune the disorder strength. In what follows $w=[0.5,2.5]$ enables the exploration of all transport regimes taking place in disordered 2D graphene and GNRQDs.

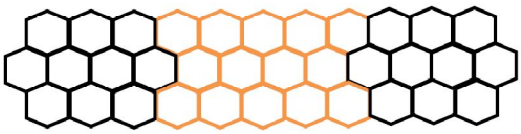

Fig. 1. Lattice configuration of GNRQD. Central region is the conductor region which is attached to two leads L and R.

In what follows, we show how to calculate the transmission of the system. In the absence of thermal effects and the charging terms, the transmission coefficient for electrons from the left lead to the right lead with energy *E* is related to Green's functions using Caroli's formula which provides high numerical accuracy and efficiency:[11], [12]

$$T = Tr(\Gamma_L G_c^r \Gamma_R G_c^a) \tag{2}$$

Where $G_c^{r,a}$ are retarded and advanced Green's functions of the conductor and $\Gamma_{R,L}$ are coupling matrices from the conductor to the leads. The systems have four leads, resulting in a conductor Green function of form:[11], [12]

$$G_c^r = \left[(E+i\eta)I - Hc - \sum_L^r - \Sigma_R^r\right]^{-1} \tag{3}$$

Where *I* is the identity matrix, Σ_R denotes the self-energy due to the coupling between the conductor and lead *R; i*η is a small imaginary term added to make the Green's function (G) non-hermitian. When there are more than two leads, the matrix algebra in (3) is somewhat more complex as described in the Reference [13]. The coupling matrices are expressed as:

$$\Gamma_R = i[\Sigma_R^{\ r} - \Sigma_R^{\ a}] \tag{4}$$

The function Γ_R is called the broadening function and describes the coupling of the device to the leads, where $\Sigma^r{}_R = (\Sigma^a{}_R)^+$.The conductor region consists of *Nc* atoms *(*where *Nc=40),* making all the matrices *Nc*×*Nc* square matrices. Integrating the transmission probability over the whole energy range and for the external bias applied to the electrodes, one can derive the tunneling current as the form:

$$I(V,T) = 2e/h \int T(V,E)[f(E-\mu_R) - f(E-\mu_L)]dE \tag{5}$$

Where *T(V,E)* is transmission probability per at the energy *E* , *f(E)* is Fermi-Dirac distribution , and *V* is the bias voltage applied to the system and μ_R (μ_L) is the chemical potential at *R(L)* lead ($\mu_R = \mu_L + eV$) . The conductance *G* (*E*) of the GNRQD can be calculated using the Landauer formula [11], [12]

$$G = (2e^2/h)T \tag{6}$$

In semiconducting materials the mean free path ℓ_e is very important quantity to assess transport efficiency of the system and the corresponding device performances, indeed ℓ_e is a physical lengths in mesoscopic transport. We note, however, that recent theoretical and experimental work have dealt with ballistic transport in mesoscopic graphene which show universal behavior in the regime where $\ell_e > W > L$, where *W* and *L* are the sample width and length [13]. Here, elastic mean-free paths is extracted numerically from the length scaling analysis of the quantum conductance by considering that, according to the considered regimes,

$$\overline{T} = N/(1 + L/\ell_e) \tag{7}$$

Where *N* is the number of active conduction channels, *L* is the length of the central conductor region; ℓ_e is the mean free path.

3. RESULTS AND DISCUSSION

The problem of disorder in systems with Dirac fermions has been studied extensively in the last few years [14, 15]. The experimental researches on graphene show that the disorder may have to be considered due to imperfect cutting and its natural specifications. It is well known that in a metal or semiconductor, disorder play an important

role: they act as scattering centers and locally modify the conduction- band. We now consider a GNRQD in the presence of random disorder, including impurities randomly concentrated in some atoms that influence the on-site energy of random atoms. It is known that electrons become localized in the presence of random disorder, a phenomena known as Anderson localization [6-8]. In the systems, random disorder localizes states, led the transmission coefficient to be decreased. Fig. 2 shows the transmission coefficient of a pure and a disordered GNRQD. The fine peaks in these curves are Van- Hov singularities (VHSs) corresponding to extreme points in the energy bands [16].The new peaks in the transmission curve correspond to the disorder states. The disorder states are quasilocalized states caused by the random disorder. The injected electron will be scattered when its energy is equal to the energy level of the quasilocalized states. In Fig. 3, we plot the mean free path of electron with different disorder density when *w=0.5*. In the presence of random disorder, *Ni* disorder are randomly distributed among *Nc* sites (where *ni=Ni/Nc*). Disorder causes electron scattering. Although scattering in graphene can be suppressed because of the symmetries of the Dirac quasiparticles, it is shown that, when its source is atomic-scale, wave functions of different symmetries can mix. When the disorder density (*ni*) is sufficiently high, so that potential field induced by different disorderes overlap, and multiscattering dominates and so this multiscatterings decreases the conductance.The strong enhancement of ℓ_e around the zero energy implies a reduced number of scattering processes. It is well known that scattering of electrons due to random disorder, at graphene device will decrease their mean free path.

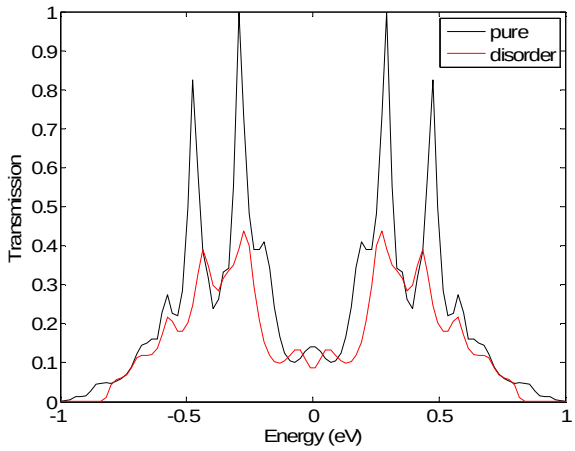

Fig. 2. The transmission coefficient of electron injected to the GNRQD; in the pure devices and in the presence of random disorder.

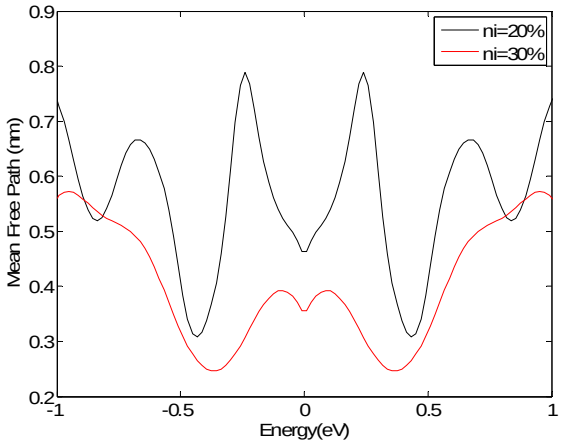

Fig. 3. The mean free path as a function of the energy *E* of the electrons with different disorder density when *w=0.5*.

In fig.4. we also show the differential conductance with different disorder density when *w=0.5*, *dI/dV*, as a function of bias voltage. We apply external potential to the system so that lead *L* lies in the potential of *V/2* and lead *R* lies in the potential of-*V/2*. The decrease of the *dI/dV* in some bias voltage means that a resistance effect appears

in this voltage. This resistance is originated from the reduced overlap between the energy bands of two leads. In some voltage the *dI/dV* increases, which means that there are conductive channels that allow the electron to pass through the central region from the *L* to the *R*. The physical reasons for this are that the system becomes unstable with bias voltage increase.

In order to investigate the behavior of changes in current voltage from lead *L* to lead *R*, and also investigating the effect of disorder on current, we apply external potential to the system. The small oscillations in the curve are due to Van-Hov singularity and originated from the "current quantization" in this mesoscopic system. According to the Fig . 5, current in the presence of disorder, decreases in comparison with the pure case, since the quasilocalized state produces additional band , in this way the electron has more channels for transport.

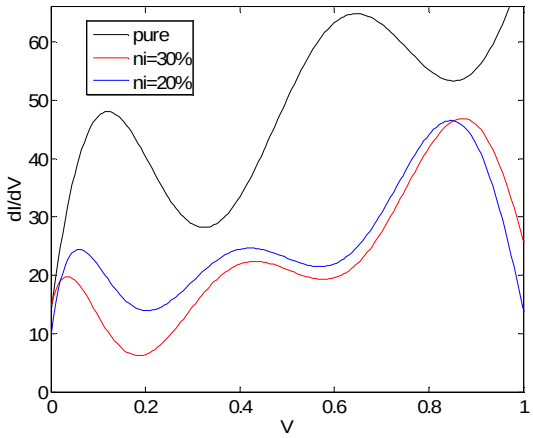

Fig.4. The conductance dI/dV as a function of bias voltage for the GNRQD, in pure case and with different disorder density

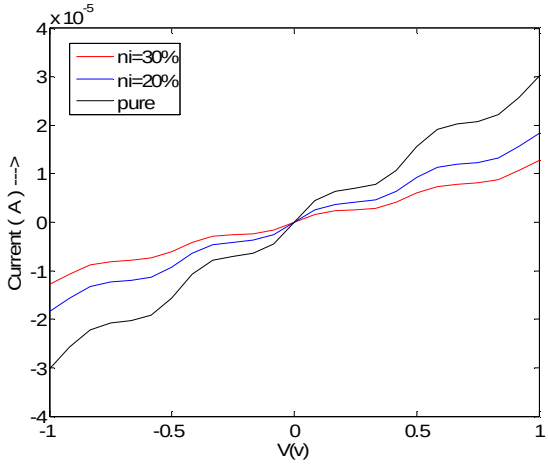

Fig. 5. Current-voltage curves of pure and disordered GNRQD

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