Conductance of T-shaped Graphene nanodevice with single disorder

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ABSTRACT: Disordered T-shaped graphene nanodevice (TGN) was designed and studied in this paper. We demonstrated the intrinsic transport properties of the TGN by using Landauer approach. Knowing the transmission probability of an electron the current through the system is obtained using Landauer-Buttiker formalism. The effects of single disorder on conductance, current and on the transport length scales are studied using tight-binding model. It is demonstrated that the transport property of the TGN depends sensitively on the disorder positions. However, the current slightly depends on the disorder sites, but strongly depends on the geometry of TGN under small bias voltage. The mean free path in the system is reduced when the strength of disorder is sufficiently high and the mean free path patterns are found to strongly depend on the disorder position. Also observe that the current basically decreases with the stem height increase. We have found that zigzag graphene nanoribbons can be used as metal leads when we build graphene nanodevice based electronic devices.

Keywords: *Landauer-Buttiker formalism; Mean free path; Single disorder; T-shaped graphene nanodevice; Transport properties.*

INTRODUCTION

Graphene sheets have the potential to be lithographed to a lot of patterned graphene nanoribbons (GNRs) to make large-scale integrated circuits. Recently, the GNR junctions with various shapes, have been investigated since the experimental realization of GNRs [1-4]. Among the rich graphene nanoribbon heterostructures, T-shaped junctions have attracted intensive attention recently [5]. Experimentally, when cutting the graphene sheet into ribbons, a certain edge roughness will always result due to the particular etching technique.Therefore, all experimentally observed graphene edges contain local defects or extended disorders.These defects aûect the electronic properties of graphene nanoribbons. Disorder effects in graphene are of particular importance on the account of its two dimensional (2D) lattice structure. In this paper we study the transport properties of disordered T-shaped graphene nanodevice (TGN) in the presence of single disorder

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using the Landauer–Buttiker approach and the tight-binding model.

EXPERIMENTAL

The geometry of T-shaped graphene nanodevice (TGN) is shown in Fig. 1. We consider the system as a central conductor region (C), connected to three leads L, R, B. Fig. 1 is the TGN junction, which is made of a metallic shoulder zigzag GNR and semiconducting stem armchair GNR. We describe the conductor and the leads by tight – binding with one π - electron per atom which is successfully used in the studies of carbon-related materials.The tight–binding Hamiltonian of the system can be written as: $H = \sum_i \varepsilon_i a_i^+ a_i + t \sum_{i,j} a_i^+ a_j$ where ε_i is on-site energy and t is the hopping matrix element between nearest neighbors. The on-site energy are taken as zero in the absence of disorder and $t = 2.78\,eV$. Also $a_i (a_i^+)$ is creation (annihilation) operator for an electron in the state on-site i .To model the single disorder, the on-site energies of one atom is distributed within the interval *[-W, W],* where *W* is the strength

of the single disorder. In what follows W= [0.5 , 2.7] enables the exploration of all transport regimes taking place in disordered 2D graphene in the presence of short range disorder. The transmission coefficient for electrons from the left lead to the right lead with energy E is [6, 7]: $T = Tr(\Gamma_m G_c^r \Gamma_n G_c^a)$ where $G_c^{r,a}$ are retarded and advanced Green's functions of the conductor and $\Gamma_{m,n}$ are coupling matrices from the conductor to the leads. The systems have three leads, resulting in a conductor- Green function of form,

$$G_c^r = \left[(E + i\eta)I - Hc - \sum_L^r - \sum_R^r - \sum_B^r\right]^{-1} \quad (1)$$

Where I is the identity matrix, Σ_n denotes the self-energy due to the coupling between the conductor and lead n. When there are more than two leads, the matrix algebra in (1) is somewhat more complex as described in the Ref [6, 7]. The coupling matrices are expressed as: $\Gamma_n = i[\Sigma_n^r - \Sigma_n^a]$, where $\Sigma_n^r = (\Sigma_n^a)^+$. The central region consists of Nc atoms, making all the matrices $Nc \times Nc$ square matrices. The average conductance of TGN can be calculated using the Landauer formula which gives us the conductance in terms of the transmission coefficients of the device: $G = (2e^2/h)\overline{T}$. Knowing the transmission probability of an electron the current through the system is obtained using Landauer-Buttiker formalism. It is written in the form [6, 7]:

$$I(V,T) = 2e/h\int T(V,E)[f(E - \mu_n) - f(E - \mu_m)]dE$$

$$(2)$$

Where $T(V, E)$ is transmission probability at the energy E, $f(E)$ is Fermi-Dirac distribution , and V is the bias voltage applied to the system and $\mu_m(\mu_n)$ is the chemical potential at $n(m)$ lead. Here, elastic mean-free paths are extracted numerically from the length scaling analysis of the quantum conductance by taking the regime under consideration into account: $\overline{T} = N_\perp/(1 + L_0/l_e)$ where $N_\perp$ is the number of active conduction channels L_0 is the sample length and ℓ_e is the mean free path length.

RESULTS AND DISCUSSION

Theorists have proposed that defects could be used to modify the electronic properties of materials, notably Graphene. Thus, in order to account for some general features of the electronic properties of the system under consideration, the single disorder is examined in three different positions in a TGN (A, B and C in Fig. 2). The conductance of the system in the presence of a single disorder in the aforementioned positions shows the modification (Fig. 3). The peaks on conductance curve of TGN result from the quasi-bound states in the TGN. In Fig. 3a we show that the presence of the disorder in the vicinity of the center of the conductor region has more impact on the conductance. However when the position of disorder is changed, the conductance decreases but remains larger than $G_0 (2e^2/h)$ since there are some states which transmit the electrons [8].
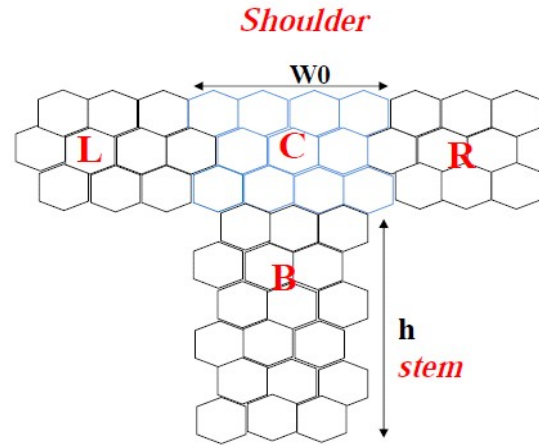

Fig. 1: Lattice configuration of T shaped graphene nanodevice (TGN). Central region is the conductor region, C, which is attached to three leads L, B and R.
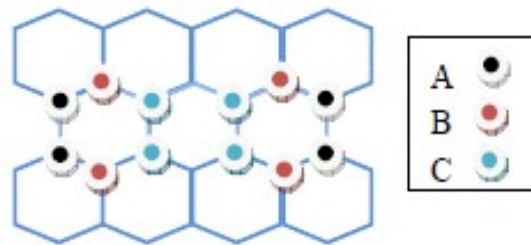

Fig. 2: Central region (conductor region), with three different single disorder positions (A, B and C).

TGN also show metallic behavior. This is also consistent with the result of the density of states (DOS) in Fig. 3b. There is a high peak near the Fermi level which is contributed by the edge states of the shoulder. It is well known that all the zigzag graphene

nanoribbons (ZGNRs) are metals at finite temperature, while all the armchair graphene nanoribbons (AGNRs) are semiconductors, so ZGNRs can be used as metal leads when we build GNR-based electronic devices [9-13].
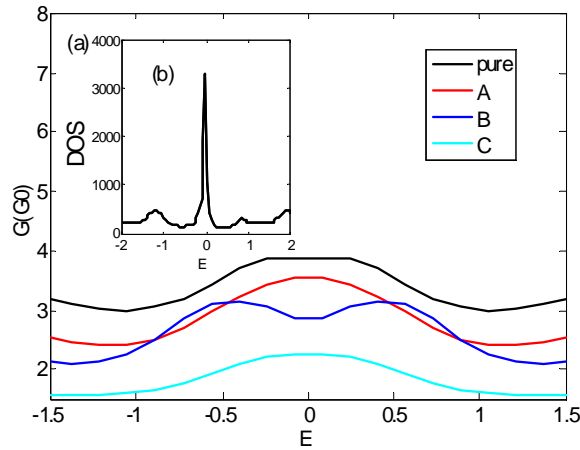

Fig. 3: The conductance of electron injected to the TGN, in pure case; in the presence of single disorder located at A, B and C sites.

An analysis of the transport length scale is examined in Fig. 4, where the mean free path is reported as a function of the energy of the electrons. Long mean-free paths for electrons near the Fermi energy are indeed originated from regular Coulomb oscillations and coherent tunneling at low temperatures and imply a reduce number of scattering processes. The mean free path patterns are found to strongly depend on the disorder position where a partial displacement of the disorder gives rise to considerable changes in scaling lengths. We may get some more information on transport length scale by studying the mean free path changes in terms of the strength of the single disorder at *E=0*. As can be seen in the inset of Fig. 4, scattering phenomenon reduces the mean free path as the strength of the single disorder gets larger, which is in a good agreement with the Fermi golden rule (FGR) $\ell_e \propto \frac{1}{W^2}$ [14].

In Fig. 5 we also show the differential conductance, *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[15-17]. 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.
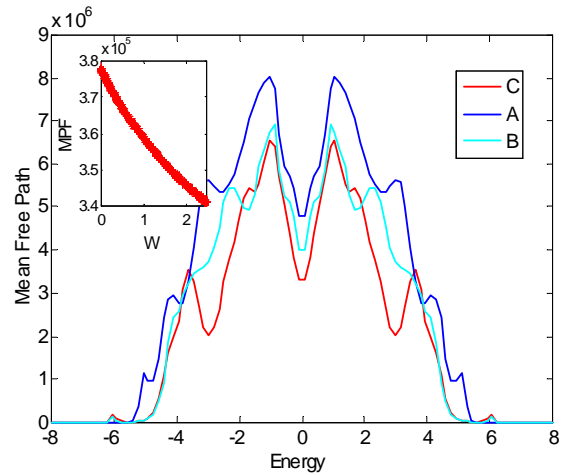

Fig. 4: Mean free path (MFP) for a TGN in the presence of single disorder located at A, B and C sites. The inset curve shows the dependence of the MFP as a function of the single disorder strength.
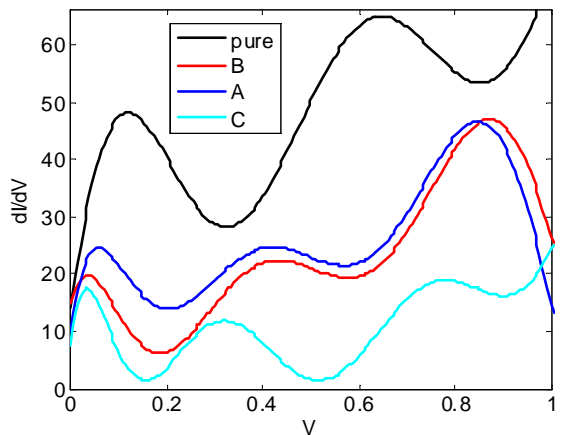

Fig. 5: The conductance dI/dV as a function of bias voltage for TGN, in pure case; in the presence of single disorder located at A, B and C sites.

Fig. 6 shows the current as a function of the height of the stem under bias voltage 0.5 *V* in the presence of single disorder located at A, B and C sites. One can note that the current presents non-monotonic behavior. Also observe that the current basically

decreases with the stem height increase. For the TGN, it has the largest values of the current, as shown in Fig. 6. The irregular vibrating behaviour is shown in Fig. 6 that the physical reasons for these observations are the quantum interference and quantum size effect [18].
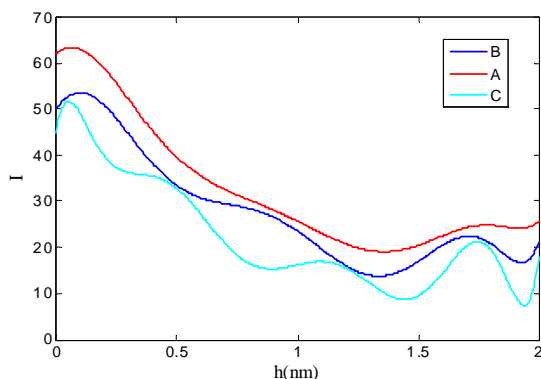

Fig. 6: The current as a function of the height of the stem under bias voltage 0.5 V in the presence of single disorder located at A, B and C sites.

CONCLUSION

A review of the effect of NPs on wettability for enhanced oil recovery processes have been presented. Several cases as well as laboratory studies were discussed. Nanotechnology has the potential to have a positive effect on the chemical EOR process. The aims of this paper were firstly to compilean up-to-date data base for wettability with NPs projects reported in the literature over the last 15 years. Altogether, nanotechnology can be an effective enhancement option for an oil recovery method in a oil reservoir which is technically sensitive to the chemical recovery method. Although the future of nanotechnology is completely uncharted territory, but certainly nanotechnology will revolutionize the oil industry in several important ways.

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