PAPER

Electronic transport in graphene nanoribbons with correlated line-edge roughness

To cite this article: Mohsen Mazaherifar et al 2019 J. Phys. D: Appl. Phys. 52 375102

View the article online for updates and enhancements.
Electronic transport in graphene nanoribbons with correlated line-edge roughness

Mohsen Mazaherifar, Ali Mojibpour and Mahdi Pourfath

School of Electrical and Computer Engineering, College of Engineering, University of Tehran, 14395-515 Tehran, Iran

E-mail: pourfath@ut.ac.ir

Received 30 March 2019, revised 24 May 2019
Accepted for publication 11 June 2019
Published 12 July 2019

Abstract

In this paper, the impact of correlation between two line-edge roughnesses (LERs) on electronic transport in armchair graphene nanoribbons (AGNRs) is investigated, employing an atomistic model based on the non-equilibrium Greens function formalism. For demonstrating the influence of this correlation, crucial transport properties like mean free path and localization lengths corresponding to different sets of roughnesses and geometrical parameters are extracted. The results indicate the substantial role of the degree of cross-correlation in transport characteristics. Besides, for showing its importance in practice, some parameters in an AGNR-based field effect transistor relating to diverse correlations are provided. Additionally, an analytical compact model is developed to formulate conductance as a function of cross-correlation coefficient. The presented results offer novel insights into electronic transport in GNRs casting light on how the correlation of LERs should be regarded as the decisive factor in choosing an experimental approach for fabrication of GNRs.

Keywords: graphene, nanoribbon, line-edge roughness, cross correlation, quantum transport, localization

(Some figures may appear in colour only in the online journal)
the roughnesses of surfaces in Si Fin, nanowires, and quantum wells has been addressed in previous studies [22–24]. The role of cross-correlation between GNR edges cannot be ignored in many cases, especially in GNRs that are produced by unzipping carbon nanotubes where both LER at both edges are fully correlated. In this study, the effect of cross-correlation between roughness of two edges of AGNRs is theoretically investigated. This paper is organized as follows: section 2 discusses the employed approach. The results are presented in section 3 and concluding remarks are presented in section 4.

2. Approach

The substitutional type is used as the model, which means carbon atoms were removed and added to the edge while the effective width was constant. This model is confirmed by experimental data [6]. Numerous samples have been developed for reducing the statistical error. Structure relaxation can be modeled by multiplying hopping parameters of π orbitals on the edge by a modifying factor [25]. However, edge bond relaxation does not affect the main purpose of the paper because its impacts are limited to the small variation in the description of band gap and curvature of subbands [3, 26, 27]. According to the aforementioned arguments, the effect of relaxation of edge atoms is ignored, since it is shown to be negligible in presence of LER. So, The electronic bandstructure of AGNRs is accurately described by a π orbital nearest-neighbor tight binding model with the coupling parameter $t = -2.7$ eV. In the utilized tight-binding model, a π covalent bond due to $p_z$-orbital was considered: $H = \sum_{\langle p,q \rangle} (\langle A_q | p_{\alpha} \rangle \langle p_{\alpha} | A_q \rangle + \langle B_q | p_{\alpha} \rangle \langle p_{\alpha} | B_q \rangle)$, where A and B represent the two atoms of graphene unit cell, $| A_q \rangle$, $| B_q \rangle$ are the atomic wave functions, $\langle p,q \rangle$ represent nearest neighbour site of p and q, and $t$ is the hoping parameter. The accuracy of this model has been previously verified [28]. In this approximate model, we do not consider electron–electron interaction. It is shown how electron–electron interaction in the presence of disorder can induce dephasing which in turn removed localized states and the transport will be in the diffusive regime. This effect is more important at high carrier concentrations and relatively long channel devices [29]. The inclusion of electron–electron interactions may affect the results, but the trends, which are the focus of this work, are not significantly affected. GNR bandstructure, density of states (DOS), and current-voltage characteristics are calculated by means of NEGF formalism [30]. The retarded Green’s function of the device is given by

$$G = [(E + i0^+)I - H - \Sigma_S - \Sigma_D]^{-1}$$

where $H$, $I$ and $E$ are the device’s Hamiltonian, identity matrix and device’s Energy, respectively, and $\Sigma_S,\Sigma_D$ designates contact self-energy at the source and drain. Surface Green’s functions are calculated based on the efficient Sancho–Rubio iteration [31].

LER is a statistical phenomenon which can be well described by means of an auto-correlation function (ACF) [32]. The number of samples in this statistical study is equal to 256 in all of the simulations. Assuming that the deviation of the width from its ideal value at some position $x_1$ is represented by $\delta W(x_1)$, the correlation between $\delta W(x_1)$ and $\delta W(x_2)$ can be described by an ACF as $R(x_1,x_2) = \langle \delta W(x_1)\delta W(x_2) \rangle$, where $\langle \ldots \rangle$ denotes statistical ensemble average. Here, an exponential ACF with zero average is used [8, 33]:

$$R(x) = \Delta W^2 \exp \left( -\frac{|x|}{\Delta L} \right)$$

where $\Delta W$ is the root mean square of the fluctuation amplitude, $\Delta L$ is the roughness correlation length, which is a measure of smoothness, and $\Delta x$ is the sampling interval chosen equal to $\alpha_x/2$, which $\alpha_x$ is the lattice constant. To create line-edge roughness in real space, we first evaluate the Fourier transform of the ACF, which gives the power spectrum of the roughness: $R(q) = \frac{\Delta W^2}{q^2} \Delta L^2$. By applying a random phase to the power spectrum followed by an inverse Fourier transform, roughness in real space is achieved [34]. LER sequences generated by using this method have zero cross-correlation coefficient [22]. To obtain two LER sequences ($Z_{up}$ and $Z_{down}$, which are the top edge roughness and bottom edge roughness, respectively) with definite cross-correlation coefficient $\rho$, Cholesky decomposition can be applied to obtain the cross-correlation matrix as follows [22]:

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ \rho & \sqrt{1-\rho^2} \end{bmatrix}$$

Thus, two random sequences $Z_{up}$ and $Z_{down}$ with a cross-correlation of $\rho$ can be expressed in terms of two un-correlated random sequences $Z_1$ and $Z_2$

$$Z_{up} = Z_1 \quad (4a)$$

$$Z_{down} = \rho Z_1 + \sqrt{1-\rho^2} Z_2 \quad (4b)$$

Fully cross-correlated (FC) edges correspond to $Z_{up} = Z_{down}$ ($\rho = 1$) and anti-cross-correlated (AC) edges correspond to $Z_{up} = -Z_{down}$ ($\rho = -1$). We have generated many samples with the same roughness parameters and have evaluated their electronic properties separately. Finally, a statistical ensemble averaging on these samples is performed.

3. Results and discussions

An AGNR composed of $N$ dimer lines is denoted as $N$-AGNR. In this work $N$ is chosen to be equal $3p$ and $3p + 1$, in which AGNRs are semiconducting materials [3] (figures 1(a)–(d)).

3.1. LDOS and transmission

The local density of states (LDOS) reads as: $D(r,E) = i/2\pi \left[ G(r,E) - G^\dagger(r,E) \right]$. Figure 1 shows the atomic structure and LDOS along two AGNRs with AC ($\rho = -1$) and FC ($\rho = 1$) edges. The maximum width variation is observed for the AC case (figure 1(a)) and because of the inverse proportionally of the band gap with the ribbon’s width, strong bandgap variation along the ribbon occurs for AC-edges (see figure 1(b)). In contrast, in the case of FC-edges, AGNR width
remains nearly unchanged (figure 1(c)) which results in nearly unaffected bandgap as depicted in figure 1(d).

The transmission probability is calculated as $T(E) = \text{trace}(\Gamma_S G \Gamma_D G^\dagger)$ with the contact broadening given by $\Gamma_{S,D} = i(\Sigma_{S,D} - \Sigma_{S,D})$. The transmission probability for AGNRs is depicted in figures 2(a) and (b) at various of correlation coefficients. The transmission corresponding to $\rho = 1$ for the 16-AGNR compared to that of the 15-AGNR follows more closely the transmission of a perfect AGNR. Nevertheless, both cases result in larger transmission probability than AGNRs with $\rho < 1$.

In figure 3, distribution of samples as a function of transmission, in energy $= 0.4$ eV, for different cross correlation coefficients is depicted. For $\rho = -1$ the distribution is right-skewed, in which the mean value is larger than median. Inversely, for $\rho = 1$ the distribution is left-skewed, in which mean value is smaller than median. However, the distribution for $\rho = 1$ is more similar to normal distribution rather than for $\rho = -1$, since the difference between mean value and median is lesser in the former. This normal-like behavior can be understood intuitively by looking at figure 3, where the distribution function for $\rho = 1$ has a cut off and beyond that cut off the probability is equal to 0, while the distribution function for $\rho = -1$ is not equipped with this cut off. Standard error is equal to standard deviation divided by the square root of number of samples. Numerous samples are used in this study in order to reduce standard error. Hence, standard errors are negligible. The extreme case of AGNRs with $\rho = -1$ can be pictured as ribbons with large roughness amplitudes resulting from concurrent fluctuation of edges. Figure 4(a) shows that the transmission steps are smeared out because of the strong distortion of the band-structure. Furthermore, the transmission is strongly suppressed because of the formation of localized states along the channel (figure 4(b)). In this regime, electron transport occurs by tunneling through these localized states and as a result the resistance exponentially decays with the length [33]. On the other hand, figures 2(c) and (d) show that in AGNRs with FC-edges the trend of the transmission of perfect AGNRs is preserved. However, a significant reduction in the transmission is observed at the beginning of the second subband. This behavior arises from the interference of localized states with a continuum at that energy and is referred to as Fano anti-resonance effect [35]. Analysis of atomistic change of LDOS allows us to further elucidate this fact: figure 4(d) depicts a mixed existence of both localized and continuum states at the energy corresponding to the beginning of the second subband that results in an anti-resonance in the transmission at this energy. LDOS, which shows the contribution of each atom to the total DOS of the lattice in the interval $[E, E + dE]$, drastically varies in space if the states in that energy interval are localized. Therefore, comparing the geometric and arithmetic averaging of LDOS over the lattice sites can provide a criterion to distinguish extended and localized states [36, 37]. The average DOS is simply given by:

$$\rho_{av}(E) = \frac{1}{K_x K_x} \sum_{i} \sum_{r} \rho_r^{i}(E), \quad (5)$$
where \( K_{s} \) is the number of samples and \( K_{s} \) is the number of sites in each sample. \( \rho_{r}(E) \) is the LDOS at some lattice site \( i \) of the \( r \)th sample at energy \( E \). The geometric average known as typical DOS is obtained from

\[
\rho_{ty}(E) = \exp \left( \frac{1}{K_{r}K_{s}} \sum_{r} \sum_{i} \ln \left( \rho_{r,i}(E) \right) \right). \tag{6}
\]

The normalized typical DOS \( R(E) = \rho_{ty}(E)/\rho_{av}(E) \), is shown in figure 2(d). For perfectly extended states, geometric and arithmetic average of LDOS become equal and \( R(E) \) reaches 1, whereas in the presence of localized states, \( R(E) \) decreases. In AGNRs with AC-edges DOS peaks at some energies corresponding to the first subband of perfect AGNR (figure 2(c)), but they are strongly localized (figure 2(d)) and do not contribute to the conduction. In the same energy range, however, GNRs with FC-edges shows larger \( R(E) \), but at the commencement of transmission steps of perfect AGNR, the states get more localized (figure 2(d)) due to excessive rate of backscattering at Van Hove singularities and give rise to Fano antiresonance seen in figures 2(a) and (b).

### 3.2. Transport length scales

To identify conduction regimes (ballistic, diffusive and localization) mean-free path \( \lambda \) and localization length \( \xi \).
presence of LER at various correlation coefficients are herein presented. Mean free path and localization length are extracted numerically from analysis of the dependence of the transmission probability on the channel length. In the diffusive and localization regimes, average transmission can be written as

\[ \langle T \rangle = \frac{N_{ch}}{1 + L/\lambda} \] and \[ \langle \ln T \rangle = -\frac{L}{\xi} \] respectively, where \( N_{ch} \) and \( L \) are the number of active conduction channels and length of the nanoribbons, respectively.

The mean free path and localization length for a 16-AGNR are depicted in figure 5. Both transport length scales strongly depend on the correlation coefficient, especially in the energy range corresponding to the first subband that dominates and determines device characteristics. In the first subband, AGNRs with FC-edges show much larger mean free path and localization lengths in comparison with AGNRs with AC-edges. However, this feature vanishes in higher subbands and the effect of correlation coefficient becomes less pronounced in higher energies. The mean free path corresponding to AGNR with FC-edges shows a dip at the beginning of the second subband due to the Fano antiresonance. Such a dip, however, is not observed in AGNR with AC-edges because of the strong bandstructure alteration in the presence of this kind of roughness.

3.3. Conductance

The ensemble average of conductance in the linear response regime as a function of correlation coefficient is sketched in figure 6. The data is fitted to the curve \( G'/(1 - \rho + \epsilon) \), where \( \rho \) and \( \epsilon \) are correlation coefficient and permittivity of nanoribbon, respectively, with a coefficient of determination (R-squared) equal to 0.93, showing that the numerical results are replicated very well by the model. Appearance of a small constant \( \epsilon = 0.02 \) in the fitted curve is due to the approximations in the assumptions (like perturbation potential and effective mass) made in the derivation. In the figure, \( G' = 0.05 \mu S \), \( L = 25 \text{ nm} \) and \( \Delta L = 3 \text{ nm} \).

The mean free path and localization length for a 16-AGNR are depicted in figure 5. Both transport length scales strongly depend on the correlation coefficient, especially in the energy range corresponding to the first subband that dominates and determines device characteristics. In the first subband, AGNRs with FC-edges show much larger mean free path and localization lengths in comparison with AGNRs with AC-edges. However, this feature vanishes in higher subbands and the effect of correlation coefficient becomes less pronounced in higher energies. The mean free path corresponding to AGNR with FC-edges shows a dip at the beginning of the second subband due to the Fano antiresonance. Such a dip, however, is not observed in AGNR with AC-edges because of the strong bandstructure alteration in the presence of this kind of roughness.

3.3. Conductance

The ensemble average of conductance in the linear response regime as a function of correlation coefficient is sketched in figure 6. The data is fitted to the curve \( G'/(1 - \rho + \epsilon) \), where \( \rho \) and \( \epsilon \) are correlation coefficient and permittivity of nanoribbon, respectively, with a coefficient of determination (R-squared) equal to 0.93, showing that the numerical results are replicated very well by the model. Appearance of a small constant \( \epsilon = 0.02 \) in the fitted curve is due to the approximations in the assumptions (like perturbation potential and effective mass) made in the derivation. In the figure, \( G' = 0.05 \mu S \), \( L = 25 \text{ nm} \) and \( \Delta L = 3 \text{ nm} \).
by $1/\tau_n(k_i) = \sum_{k'_i} S_n(k_i, k'_i)(1 - |\langle k'_i/k_i \rangle| \cos \alpha)(1 - f(k'_i))$, where $\alpha$ is the angle between initial and final wave-vector and $S_n(k_i, k'_i) = (2\pi/\hbar)|\langle \psi_n(k'_i)||H_{\text{LER}}||\psi_n(k_i) \rangle|^2 \times \delta(E_n(k'_i) - E_n(k_i))$ is the transition rate of electrons due LER scattering from initial wave-vector $k_i$ to final wave-vector $k'_i$ calculated through Fermi’s golden rule [8]. Here, we assume a smooth LER with a perturbation potential $H_{\text{LER}} = -E_{\text{c},n}\delta W/W$, where $E_{\text{c},n}$, $\delta W$ and $W$ are band-edge energy of subband $n$, width fluctuation and average width of the ribbon, respectively. With a similar calculation as [8], it is straightforward to show that the ensemble average of the square of transition matrix elements $M_n(k_i, k'_i) = \langle \psi_n(k_i) ||H_{\text{LER}}||\psi_n(k_i) \rangle$ can be calculated as:

$$|M_n(k_i, k'_i)|^2 = \left( \frac{E_{\text{c},n}}{W L} \right)^2 \int \langle \delta W(x_1) \delta W(x_2) \rangle$$

$$\exp \left[ -iq(x_1 - x_2) \right] dx_1 dx_2$$

(7)

where $q = k_i - k'_i$. Noting that $\delta W(x) = Z_{\text{Up}} - Z_{\text{Down}}$ and employing equation (4a) and considering $\langle Z_1(x_1)Z_2(x_2) \rangle = \langle Z_2(x_1)Z_2(x_2) \rangle = R(x)$ (see equation (2)), one can simplify the integrand as:

$$\langle \delta W(x_1) \delta W(x_2) \rangle = 2(1 - \rho)R(x)$$

(8)

In the derivation of equation (8), a zero cross-correlation between $Z_1$ and $Z_2$ is assumed, i.e. $\langle Z_1(x_1)Z_2(x_2) \rangle = 0$. The variable $1 - \rho$ is independent of energy, wave-vector and position and therefore comes out of integrals over these variables. The conductivity is therefore $\sigma \propto 1/(1 - \rho)$.

### 3.4. Roughness and geometrical parameters

The ensemble average transmission for two values of correlation length at various correlation coefficients are depicted in figures 7(a) and (b). A small value of correlation length results in a clear separation of FC and AC-edge transmission curves. As the correlation length increases, AGNR becomes less sensitive to the value of correlation coefficient and transmission curves become indistinguishable which is clearly observed in figure 7(c). In fact, LER becomes smoother with the correlation length, which makes scattering rate smaller and results in the convergence of transmission probabilities of AGNRs to that of an AGNR with perfect edges.

The ensemble average of the value of transport gap, which is defined as the energy interval at which transmission probability falls below 0.01, for AGNRs with FC and uncorrelated edges is sketched in figure 7(d). Numerical analysis shows that the transport gap of FC-edge AGNR is equal to the value of band gap for all values of correlation length. In contrast, in uncorrelated edge AGNR, transport gap is larger than the band gap of perfect AGNR for correlation lengths below 8 nm.

The ensemble average of the transmission probability decrease as the roughness amplitude increases. As depicted in figure 8(a), AGNRs with AC-edges are more sensitive to the change in roughness amplitude than AGNRs with FC-edges. While the transmission probability is nearly the same for AGNRs with FC and AC-edges at small roughness amplitudes, they deviate as the roughness amplitude increases. The effect of roughness amplitude is further elucidated by considering its
effect on the transport gap. As shown in figure 8(b), the transport gap increases with the roughness amplitude for AGNRs with AC-edges, whereas it remains nearly constant in the case of AGNRs with FC-edges. Figure 8(c) depicts the variation of the ensemble average transmission probability as a function of the length. In long ribbons, especially when the electronic system is in the localization regime, the effect of correlation between edges is pronounced and AGNRs with FC-edges show an order of magnitude larger transmission probabilities than AGNRs with AC-edges. This behavior is due to the fact that in longer ribbons, electrons experience more scattering.

The effect of ribbon’s width on the transport gap of AGNR with correlated edges is investigated in figure 8(d). Wider AGNRs are more robust to LER [7]. This robustness leads AGNRs with AC-edges to show similar transport gaps as AGNRs with FC-edges in wide ribbons.

### 3.5. Device characteristics

The role of edge roughness correlation on GNR based FETs is herein investigated. The transport equations are self-consistently solved the Poisson equation until a convergence criterion is satisfied. More details are provided in [30, 39]. The drain current $I_D$ can be calculated as $I_D = (2q/h) \int T(E) f_S(E) - f_D(E) dE$, where $q$ and $h$ are electron charge and planck’s constant, respectively, and $f_S, f_D$ denotes Fermi–Dirac distribution function in the source and drain regions. The drain-to-source voltage, $V_{DS}$, is equal to 0.5 and the Fermi levels at the source and drain contact are set to 0.1 eV above conduction band. In order to explore the effect of correlated edge roughness on the device characteristics, $I_D - V_G$ of 16 and 28-AGNRs are shown in figures 9(a) and (b). In both cases, AGNRs with FC-edges show larger $I_{on}$ (on-state current) and a smaller $I_{off}$ (off-state leakage current). Figure 9(c) shows the behavior of $I_{on}$ and $I_{off}$ for 16-AGNRs in more detail. The reduction of the correlation coefficient results in an increase in localized mid-gap states. These states facilitate the tunneling of carriers through the barrier and increase the off-current (figures 9(f) and (e)). The off-current increases in AGNRs with AC-edges by two orders of magnitude compared to the AGNRs with FC-edges. In addition, roughness correlation reduces the on-current of AGNRs with AC-edges because of excessive scattering rate. Figure 9(d) depicts the enhancement of the current on/off ratio for 16-AGNR with the correlation coefficient.

The subthreshold swing and transconductance are the other important figures of merit for FETs which are defined as $S = \partial V_G / \partial \log I_D$ and $g_m = \partial I_D / \partial V_G$. Figure 10(a) shows a decrease in the sub-threshold swing for a 28-AGNR as correlation coefficient increases. The values should be compared with 60 mV dec$^{-1}$, which is the sub-threshold swing of an ideal FET at room temperature. Furthermore, transconductance also increases 300 percent as the correlation coefficient increases.

![Figure 8](image_url)

**(Figure 8)**. (a) The average transmission probability at $E = 0.6$ eV as a function of roughness amplitude at various correlation coefficients. (b) The average transmission as a function of energy and roughness amplitude for 16-AGNRs with AC and FC-edges. The transport gap is depicted by dash lines. (c) The average transmission at $E = 0.7$ eV as a function of AGNR length at various correlation coefficients. (d) The transport gap as a function of AGNR width. In order to clearly show the trend only $(3p)$-AGNRs (where $p$ is an integer) is shown in (d), but the same trend holds for $(3p+1)$-AGNRs. For (a)–(c) 16-AGNR is assumed. In all figures, $L = 20$ nm and $\Delta L = 3$ nm.
Figure 9. The ensemble average of the transfer characteristics at various correlation coefficients for (a) 16-AGNR, (b) 28-AGNR. The average (c) $I_{\text{on}}$ and $I_{\text{off}}$, and (d) the average of the current on/off current ratio as a function of the correlation coefficient for 16-AGNRs. (e), (f) Spatially resolved local density of states (LDOS) projected on the position of AGNRs in its off-state. The solid lines show conduction and valance bands. For 16-AGNRs $L = 20$ nm, for 28-AGNRs $L = 25$ nm and in all figures $\Delta W/W = 2\%$.

Figure 10. The ensemble average of the (a) sub-threshold swing and (b) transconductance as a function of correlation coefficient for 28-AGNRs. In all figures, $\Delta W/W = 2\%$ and $\Delta L = 3$ nm.
from $-1$ to $1$ (see figure 10(b)). These enhanced characteristics are direct consequences of increased $I_{\text{on}}$ and reduced $I_{\text{off}}$ as the structure moves from AC-edges to FC-edges.

4. Conclusions

By using NEGF formalism along with an atomistic tight-binding model, it is shown that the ignored effect of correlation between rough line-edges of AGNRs has a significant impact on the electronic transport. An electron transport fingerprint is identified in the FC-edge AGNR caused by Fano antiresonance. The normalized typical DOS is calculated and used to quantitatively analyze localized and extended states. The results show that localized states and a continuum coexist at commencement of new subbands leading to Fano antiresonance. Narrow AGNRs with FC-edges show more than 10-fold longer mean free path and localization lengths at energies corresponding to the first subband in comparison to AGNRs with AC-edges. Next, an analytical calculation capturing the $1/(1 - \rho)$ behavior of conductance is presented. Finally, FETs based with correlated line-edge roughness are analyzed and have shown more than four orders of magnitude increase in the on/off current ratio, nearly ideal sub-threshold swing and four times larger transconductance in AGNRs with FC-edges in comparison with that of AGNRs with AC-edges. The presented results explain the significant superior performance of GNDRs that are obtained from unzipping of nanotubes (FC-edges) in comparison with that of GNDRs which are obtained from other methods where edge roughnesses are not correlated.

ORCID IDs

Mahdi Pourfath @ https://orcid.org/0000-0002-8053-578X

References

[34] Wu J 2004 Tribol. Int. 37 339–46
[35] Miyoshinchenko A E, Flach S and Kivshar Y S 2010 Rev. Mod. Phys. 82 2257
[37] Zare M, Amini M, Shahbazi F and Jafari S 2010 J. Phys.: Condens. Matter 22 255503
[38] Cresti A and Roche S 2009 Phys. Rev. B 79 233404