Student Paper

Effects of Correlated Edge Roughness on the Electronic Properties of Armchair Graphene Nanoribbons

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Graphene is gapless material. To employ it for electronic applications a finite energy gap needs to be induced. This can be achieved by patterning graphene into narrow nanoribbons, where carriers are physically confined along the transverse direction. The induced gap is inversely proportional to the width of the ribbon. To obtain suitable band-gaps for digital applications, the width of the ribbons should be in the order of a few nanometers. In narrow graphene nanoribbons (GNRs), however, edge roughness is the dominant scattering mechanism [1]. The effects of edge roughness on the electronic property of GNRs have been widely studied [1-2]. However, the correlation between rough edges has been neglected so far. In GNRs obtained from patterning of graphene, rough edges are nearly uncorrelated. One of the well-established methods for obtaining GNRs with smooth edges is unzipping of carbon nanotubes [3], where rough edges are fully cross-correlated. This indicates the need for a careful study of the role of cross-correlation between rough edges on the electronic properties of armchair GNRs (AGNRs). In this work, we present for the first time a comprehensive study on the importance of the degrees of correlation between rough edges of GNRs.

The non-equilibrium Green's function (NEGF) [2] along with a tight binding model for describing the electronic band-structure is employed [4] to investigate electronic transport of carriers in AGNRs in the presence of correlated edge roughness. A stochastic approach is used to model edge roughness, where an exponential auto-correlation between edge fluctuations is assumed [2]:

$$R(x) = \Delta W^{2} \exp(-x/\Delta L) \qquad (1)$$

Here, ΔL is the roughness correlation length which is a measure of smoothness and ΔW is the root mean square of the fluctuation amplitude. Edge roughness in real space can be obtained by adding a random phase to the power spectrum of the auto-correlation followed by an inverse Fourier transform [2]. Using this method two uncorrelated roughness profiles z_1 and z_2 are generated. Correlated roughness profiles can be created by considering the cross-correlation coefficient ρ which varies between -1 and 1. The roughness profiles of the upper and lower edges are therefore given by:

$$z_{up} = z_1, z_{down} = \rho z_1 + \sqrt{1-\rho^2}\, z_2, \qquad (2)$$

Fig. 1 shows the sketch and the local density of states (LDOS) along the AGNRs with two extreme values of the cross-correlation coefficient. For anti-cross-correlated edges ($\rho = -1$) the maximum width variation is observed (Fig. 1(b)). Because of the width-dependence of the bandgap, this translates into strong variation of the bandgap for anti-cross-correlated rough edges, see Fig. 1(b). On the other hand, in the case of the fully cross-correlated edges ($\rho = 1$) the GNR width remains nearly constant (Fig. 1(c)) and as a result the bandgap is only weakly affected, see Fig. 1(d).

The transmission probability as a function of energy at various cross-correlation coefficients is shown in Fig. 2(a). The largest transmission probability is observed for the AGNR with fully cross-correlated edges. In this case, because of nearly constant bandgap along the channel, the carrier scattering rate is minimum and the mean free path (MFP) of carrier is larger than that of AGNRs with smaller cross-correlation coefficients, see Fig. 2(b). On the other hand, in the case of anti-cross-correlated edges, due to maximum width variation along the channel the scattering rate is relatively large and the MFP is the smallest one.

The transmission probability as a function of length is shown in Fig. 2(c). For short channel lengths, the transport of carriers is diffusive, whereas for longer channel lengths localization of carriers

occurs [2,5]. In a phase-coherent channel, at long channel lengths, the incident and reflected wave functions (due to disorder) form localized states along the channel and carriers are transferred by hopping between these localized states. In this regime the transmission probability decreases exponentially with the length [2,5]. Fig. 2(c) indicates that the effect of the cross-correlation between rough edges is more pronounced in the localized regime than in the diffusive regime. Due to the absence of various phase breaking scattering mechanisms in AGNRs, such as electron-phonon interaction, carrier transport is phase-coherent [6] which allows the formation of localized states along the channel. In AGNRs with anti-cross-correlated rough edges the bandgap varies frequently along the channel, which in turn causes the reflection of carriers and formation of more localized states along the channel. In the other extreme with fully cross-correlated edges, because of relatively small number of reflections, few localized states are formed and significantly larger transmission probabilities are observed.

In summary, the effect of cross-correlation between rough edges of AGNRs is investigated in this work. In AGNRs with fully cross-correlated edges the transmission probability and the MFP are larger than in those with smaller cross-correlation coefficients. Additionally, the effect of cross-correlation is more pronounced in the localization regime.

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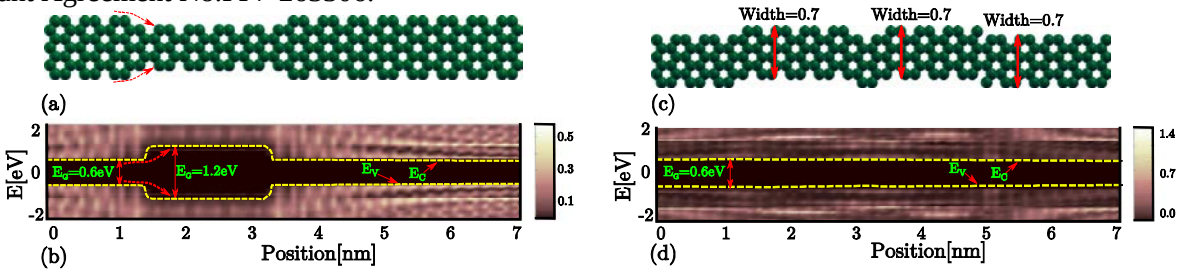

Fig. 1. The schematic and the LDOS for AGNRs with (a), (b) anti cross-correlated edge profiles ($\rho = -1$) and with (c), (d) fully cross-correlated ($\rho = +1$)

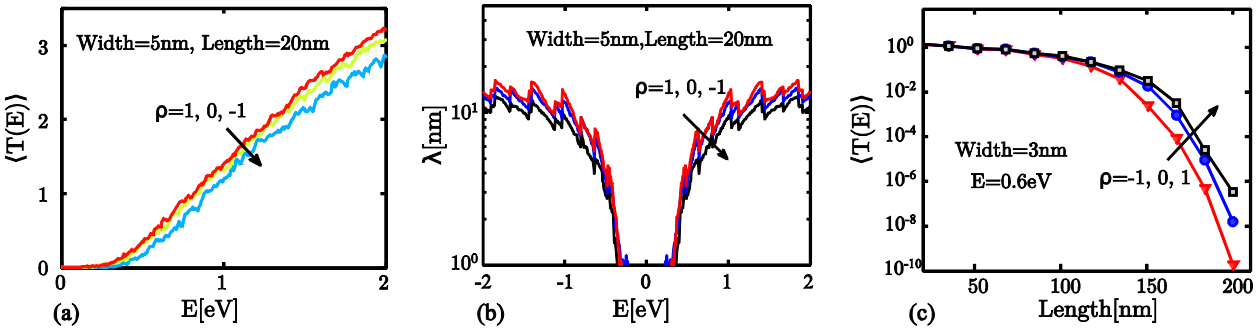

Fig. 2. (a) The average transmission probability as a function of energy at various cross-correlation coefficients. (b) The mean free path as a function of energy at various cross-correlation coefficients. (c) The dependence of the transmission probability on the channel length at various cross-coefficients. (ΔL=3nm, ΔW/W=6%)

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