Electronic Transport in Graphene Nanoribbons in the Presence of Substrate Surface Corrugation

S. B. Touski*, M. Pourfath*† H. Kosina†
*School of Electrical and Computer Engineering, University of Tehran, P.O.BOX 14395-515, Tehran, Iran
†Institute for Microelectronics, Technische Universität Wien, Gußhausstraße 27–29/E360, A-1040 Wien, Austria
pourfath@iue.tuwien.ac.at

Graphene is a two-dimensional material which has attracted the attention of many scientists over the past few years. To use graphene for electronic applications it should be placed on a substrate. The surface of any substrate has always a degree of corrugation. Substrate surface corrugation affects the surface morphology which in turn modulates the electronic properties of devices placed on such substrates. In this work the role of surface corrugation parameters on the electronic properties of armchair graphene nanoribbons (AGNRs) is studied, employing the non-equilibrium green's function formalism along with a tight-binding description of the electronic bandstructure. The mean free path as functions of the geometrical and corrugation parameters is extracted and discussed.

Surface corrugation affects the bonding lengths between carbon atoms which in turn modulates the hopping parameters [1]. Pereira and co-workers used a rate of decay $dt_{ij}/dl = -6.4\text{eV/Å}$ and proposed an exponential dependence of the hopping parameter on the bonding length [2, 3]:

$$t_{ij}(l) = t_0 \exp\left[-3.37\left(l/a_{cc} - 1\right)\right] \qquad (1)$$

$a_{cc} = 0.142$nm is the bonding length at equilibrium and l is the bonding length in the presence of strain or corrugation. The small bending of p_z-orbitals due to corrugation has only a weak effect. It has been shown that the effect of the hopping parameter modulation due to bonding length variation dominates that of orbital bending [4].

Surface corrugation of the substrate is a statistical phenomenon which can be modeled by a Gaussian auto-correlation function (ACF) [5, 6]:

$$R(x,y) = \delta h^2 \exp\left(-\frac{x^2}{{L_x}^2} - \frac{y^2}{{L_y}^2}\right) . \qquad (2)$$

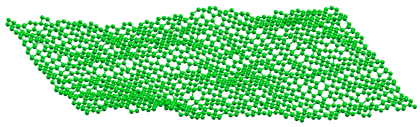

Fig. 1. 3D sketch of a corrugated AGNR.

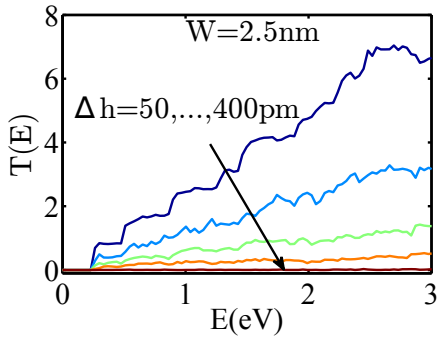

Fig. 2. The average transmission probability as a function of energy at various corrugation amplitudes. $W = 2.5$nm, $L = 100$nm, and $L_x, L_y = 25$nm.

L_x and L_y are the correlation lengths along the x and y-direction, respectively, and δh represents the root mean square of height fluctuations. To generate surface corrugation in the spatial domain (see Fig. 1) the ACF is Fourier transformed to obtain the spectral function. A random phase is applied and the achieved function is inverse Fourier transformed [7]. Using this method many devices are created for a given set of geometrical and corrugation parameters. Each sample is simulated separately followed by taking the ensemble average of the results.

The average transmission probability as a func-

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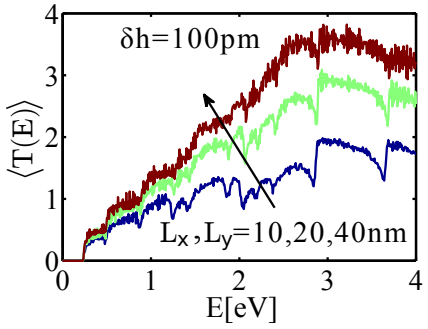

Fig. 3. The average transmission probability at various correlation lengths. $W = 2.5$nm, $L = 85$nm, and $\delta h = 50$pm.

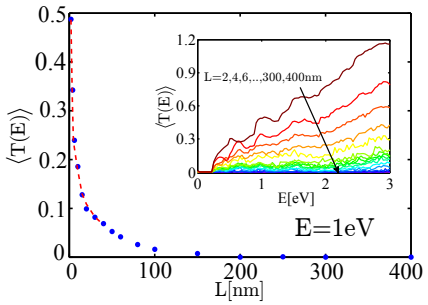

Fig. 4. The average transmission probability as function of length at $E = 1$eV. $W = 2.5$nm , $L_x, L_y = 15$nm, and $\delta h = 250$pm. The dashed-line is a fitted curve for extracting the MFP.

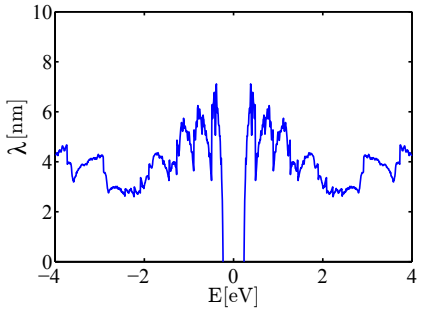

Fig. 5. The mean free path as a function of energy. $W = 2.5$nm, $L_x, L_y = 15$nm, $\delta h = 150$nm.

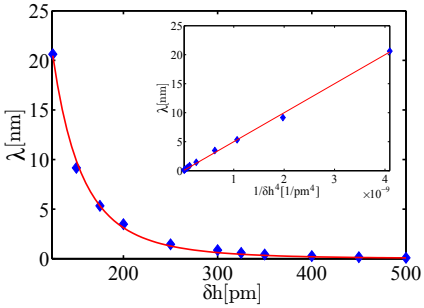

Fig. 6. The dependency of the MFP on the corrugation amplitude. The inset indicates that the MFP scales as $\lambda \propto \delta h^{-4}$. $L_x = L_y = 15$nm, $W = 5$nm.

tion of energy for different δh is shown in Fig. 2. As corrugation amplitude increases the transmission probability decreases due to an increased carrier scattering rate. On the other hand, the average transmission probability increases with the corrugation correlation length, see Fig. 3. A larger correlation length implies a smoother height variation which results in smaller bonding length modulation.

To quantify the role of surface corrugation on the electronic properties of AGNRs the mean free path (MFP) as function of the corrugation parameters can be investigated. In the diffusive transport regime the transmission is inversely proportional to the channel length:

$$T(E) = N_{\rm ch}(E)/(1 + L/\lambda(E)) \ , \qquad (3)$$

where $\lambda(E)$ represents the MFP of carriers. To extract the MFPs at each energy a curve based on Eq. (3) is fitted to the average transmission probability as a function of the channel length (Fig. 4) and the respective MFP at that particular energy is numerically extracted (Fig. 5). The MFP as a function of energy for $\delta h = 150$pm is shown in Fig. 6. The results indicate that the MFP scales as $\lambda \propto \delta h^{-4}$ with the corrugation amplitude.

Depending on the material type and cleaning process, typical values the corrugation amplitude are $168 - 360$pm, 75pm, and 24pm for SiO_2, Boron-Nitride, and Mica, respectively [6, 8]. Although smooth surfaces of Boron-Nitride and Mica substrates are better suited for graphene based devices, SiO_2 is more widely used in microelectronics. Therefore, the analysis of graphene based devices on SiO_2 substrates requires a careful study of the role of substrate corrugation on the electronic transport.

References

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