Spin Transport in Graphene Nanoribbons: The Role of Surface-Corrugation

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***Abstract*— Spin-orbit interaction in flat graphene is rather weak due to the symmetry of the lattice. However, substrate surface-corrugation can break this symmetry and induce a relatively large spin-orbit interaction. In this work we study spin transport in armchair graphene nanoribbons (AGNR) in the presence of substrate surface-corrugation. We employ the non-equilibrium green's function along with a multi-orbital tight-binding model. The role of corrugation amplitude on the spin transmission probability and polarization has been investigated.**

Due to the low atomic number of carbon, spin-orbit coupling in graphene is weak and theoretically a spin relaxation time of about micro- to millisecond is expected[1]. Experimental studies, however, indicate spin relaxation times in the range of $100 - 200$ps [2] which are much shorter than the theoretically predicted ones. On the one hand graphene should be placed on a substrate to be used for electronic applications. On the other hand the surface of the substrate is not perfect and can have some degrees of roughness. Surface-corrugation induced curvature can significantly increase spin-orbit interaction in graphene [3] which in turn affects spin-relaxation time in this material. The role of surface-corrugation on the electronic charge transport has been studied in Refs. [4], [5]. In this work, for the first time, an atomistic multi-orbital Hamiltonian along with the non-equilibrium Green's function formalism are employed to study the role of surface-corrugation on spin transport in AGNRs. The electronic bandstructure of graphene is described by a nearest neighbor tight-binding model with three orbitals p_x, p_y, p_z. The hopping parameters are $t_{sp\sigma} = +5.580$eV, $t_{ss\sigma} = -6.769$eV, $t_{pp\sigma} = +5.037$eV, $t_{pp\pi} = -3.033$eV [6]. Substrate surface-corrugation modulates bonding lengths and as a result the hopping parameters. The variation of the hoping parameters with the bonding length is considered using Harrison's model $t_{ij} \propto 1/d^2$. In addition, bonding directions are also altered in the presence of surface-corrugation, which can be modeled by the Slater-Koster approach [7]. On the other hand, spin-orbit interaction is considered by including the spin-orbit Hamiltonian defined as $H_{\rm SO} = \Delta \hat{L} \cdot \hat{S}$ where $\Delta = 12$meV is the intra-atomic spin-orbit coupling constant, $\hat{L}$, and $\hat{S}$ are the atomic angular momentum and spin operators, respectively. Because of the lattice symmetry in a flat graphene sheet, the spin-orbit interaction is nearly negligible. However, in the presence of substrate disorder this symmetry is broken and spin-orbit interaction is considerably increased.

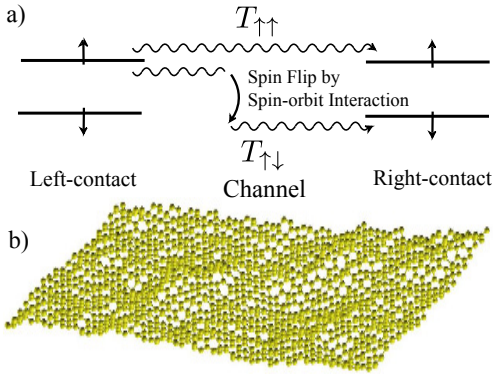

Fig. 1. (a) Spin transport and the related transmission probabilities in the presence of spin-flip mechanisms and (b) the surface of a corrugated graphene.

The transmissions probability for electrons from the left-contact with up-spin to the right-contact with up-spin is defined as $T_{\uparrow\uparrow} = T_{\uparrow\uparrow} = \mathrm{Trace}[\Gamma_{L\uparrow} G_{\uparrow\uparrow} \Gamma_{R\uparrow} G^{\dagger}_{\uparrow\uparrow}]$, while the transmission

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from the left-contact with up-spin to the right-contact with down-spin and is denoted by $T_{\uparrow\downarrow} = T_{\uparrow\downarrow} = \text{Trace}[\Gamma_{L\uparrow} G_{\uparrow\downarrow} \Gamma_{R\downarrow} G^{\dagger}_{\uparrow\downarrow}]$, see Fig. 1(a). $\Gamma_{L,\uparrow,\downarrow}$ and $\Gamma_{R,\uparrow,\downarrow}$ are the broadening associated with the left- and right-contact, the components of the Green's function are given by

$$\begin{pmatrix} G_{\uparrow\uparrow} & G_{\uparrow\downarrow} \\ G_{\downarrow\uparrow} & G_{\downarrow\downarrow} \end{pmatrix} = \Big[EI - \begin{pmatrix} H_{\uparrow\uparrow} & H_{\uparrow\downarrow} \\ H_{\downarrow\uparrow} & H_{\downarrow\downarrow} \end{pmatrix} - \begin{pmatrix} U_{\uparrow} & 0 \\ 0 & U_{\downarrow} \end{pmatrix} - \begin{pmatrix} \Sigma_{L\uparrow,R\uparrow} & 0 \\ 0 & \Sigma_{L\downarrow,R\downarrow} \end{pmatrix} \Big]^{-1}$$

Surface-corrugation of the substrate is an statistical phenomenon which can be modeled by a Gaussian auto-correlation function (ACF) $R(x,y) = \delta h^2 \exp\left(-x^2/L_x^2 - y^2/L_y^2\right)$ [8] where L_x and L_y are the roughness correlation lengths along the x and y-direction, respectively, and δh is the root mean square of the height fluctuations. To generate roughness in the spatial domain, a random phase is added to the power spectrum of the auto-correlation function followed by an inverse Fourier transform [4], see 1(b). For any set of geometrical and roughness parameters many devices are generated. Finally, the characteristics of each device is evaluated and followed by an ensemble average over all structures.

To study the effect of substrate surface-corrugation on spin transport, an spin-up polarized current is injected to the left-contact. In the presence of spin-orbit interaction the spin of some electrons flips and both up- and down-spin electrons can be founded at the right-contact. $T_{\uparrow\downarrow}$ and $T_{\uparrow\uparrow}$ are plotted as a function of energy at various corrugation amplitudes in Fig.2(a) and (b), respectively. Because of increased scattering, $T_{\uparrow\uparrow}$ decreases with the increase of the surface-corrugation amplitude. Although one could expect that $T_{\uparrow\downarrow}$ increases with the surface-corrugation amplitude, the results do not confirm this trend. This behavior can be understood by noting that $T_{\uparrow\downarrow}$ is affected by two opposing effects. On the one hand the increase of the roughness amplitude results in the increase of the spin-orbit constant and thus in increased spin-flipping. On the other hand corrugation like other scattering mechanism reduces the transmission probability. At large roughness amplitudes the latter dominates. Fig.3 shows the polarization efficiency as a function of energy at various surface-corrugation amplitudes.

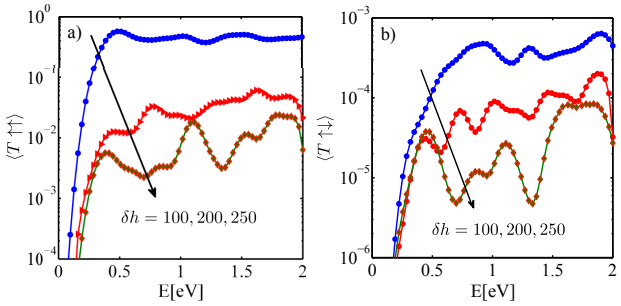
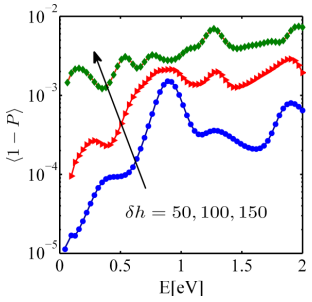


Fig. 2. An ensemble average of (a) $T_{\uparrow\uparrow}$ and (b) $T_{\uparrow\downarrow}$ as functions of energy at various corrugation amplitudes.$W = 2nm$, $L = 25nm$ and $L_x, L_y = 10nm$.



3. An ensemble average of $1 - P$ as a function of energy at various substrate surface-corrugation amplitudes. The polarization efficiency is defined as $P = (T_{\uparrow\uparrow} - T_{\uparrow\downarrow})/(T_{\uparrow\uparrow} + T_{\uparrow\downarrow})$ [9] W = 2nm, L = 25nm and $L_x, L_y = 10nm$.

The results indicate that the polarization decreases with the surface-corrugation. This behavior, which is in agreement with the results of Refs. [3], [10], is due to increased spin-orbit interaction in the presence of surface-corrugation. The results indicate the important of including surface-corrugation for accurate modeling of graphene-based spintronic devices. The effect of surface-corrugation on spin transport in AGNRs is theoretically investigated. Because of the symmetry breaking in graphene lattice by substrate surface-corrugation, both the $T_{\uparrow\uparrow}$ and $T_{\uparrow\downarrow}$ are reduced in the presence of this type of disorder, whereas the polarization decrease as the surface-corrugation amplitude increases.

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