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The effect of line-edge roughness on the electronic properties of graphene nano-ribbons

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Graphene, a one-atomic carbon sheet with a honeycomb lattice, has attracted significant attention due to its unique physical properties [1]. This material shows an extraordinarily high carrier mobility of more than 100,000 cm²/Vs [2] and is considered a major candidate for a future channel material for high performance transistors [3]. To induce an electronic bandgap, a graphene sheet can be patterned into narrow ribbons. In order to obtain an energy bandgap larger than 0.1 eV, which is essential for electronic applications, the width of the graphene nanoribbon (GNR) must be scaled below 10nm. In this regime line-edge roughness is the dominant scattering mechanism. Applying a tight-binding model, the effect of line-edge roughness is studied. To model transport of carriers in GNRs the non-equilibrium Green's function (NEGF) formalism is employed. The NEGF method appears to be the most appropriate model for nanoscale devices [4]. In this formalism quantum effects, such as tunneling, size quantization, and quantum interference of carriers are included. Quantum mechanical collisional effects in the scattering of carriers, such as collisional energy broadening, are also properly modeled.

The line-edge roughness can be trated perturbatively [5]. However, in a more accurate non-perturbative approach one can consider the roughness as a stochastic phenomenon and realize it by removing or replacing specific carbon atoms located at the edges of the ribbon. In order to model roughness, an exponential auto-correlation function is used [6]. In the model the roughness is described by an amplitude $\Delta_{\rm m}$ and a correlation length $L_{\rm m}$. The stochastic roughness can be generated by applying a random phase to the power spectrum of the roughness autocorrelation in the Fourier domain followed by an inverse Fourier transform in order to obtain the roughness in the real space domain. Fig. 1 shows the spatial distribution of the current amplitude

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along a GNR with rough edges. Due to multiple scattering of carriers between the two rough edges, a large circulating current is present at some locations inside the channel. Furthermore, the atomistic tight-binding model can capture the granularity of the simulation domain, which is essential for narrow GNRs. To investigate the effect of roughness on the current of GNRs, one can consider the ratio of the current in the presence of roughness to that of a GNR with perfect edges, $R_{Rough} = I_{Rough}/I_{Perfect}$. Fig. 2 shows R_{Rough} as a function of the GNR width. As the width of the ribbon decreases the current decreases. However, for very narrow ribbons lineedge roughness results in strong localization of carriers. In this regime the resistance of the channel increases exponentially and the current considerably decreases. The results indicate the importance of employing atomistic quantum mechanical simulations for an accurate analysis of nanoscale devices.

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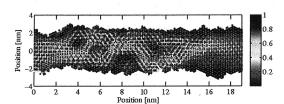


Figure 1: Spatial distribution of the normalized current amplitude along a GNR with line-edge roughness. The ribbon's length is 19nm and the width is 5nm. An exponential auto-correlation for line-edge roughness has been assumed. The roughness is described by a correlation length of L_m =3nm and an amplitude of Δ_m =2 a_m :

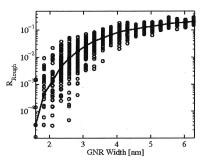


Figure 2: Current reduction due to line-edge roughness as a function of the ribbon's width. The roughness amplitude is $\Delta_m = 4a_{c'}$.