Design of graphene electronic devices using nanoribbons of different widths

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(Received 25 August 2009; accepted 12 October 2009; published online 5 November 2009)

We present a simple design of a field effect transistor based on graphene nanoribbons, taking advantage of the metallic and semiconductor nature of nanoribbons with different widths. Such device could be constructed by using lithography techniques. The conductance of the proposed device is obtained by using the Kubo formula, assuming a strong damping due to the substrate and imperfections of the lattice. By removing the control electrodes, the design could also be used as an electrical resistance. © *2009 American Institute of Physics*. [doi:10.1063/1.3257731]

Graphene is considered as a material with fascinating properties.[1–4] As an example, electrons in graphene behave as massless relativistic fermions[5–8] due to its conical dispersion relation.[9,10] The carrier mobility is very high, and remains higher even at high electric fields.[11] Therefore, graphene seems to be a promising material for building electronic devices which eventually could lead to "carbon computers," although there are some problems that need attention such as the Klein effect, which make difficult the control of electronic transport.[2] In fact, in order to produce electronic devices like a field effect transistor (FET), one needs to control the conductivity by using gates. In graphene, gates have been constructed using quantum dots,[3] and in a previous paper, we have demonstrated that a possible way to control electrons is by inducing a metal-insulator transition with substitutional doping atoms.[12] Such an idea has been confirmed recently using angle-resolved photoemission spectroscopy.[13] Electromagnetic radiation could also be used to produce mass in the otherwise zero mass carriers.[14] However, if one has in mind the idea of building integrated circuits, it is better to use graphene lithography,[15] but this technique still shows some difficulties on of how to "stop" electrons in graphene. Here we present the idea of using nanoribbons of different widths to build gates and resistors, due to the fact that graphene nanoribbons could behave as either semiconductors or metals depending on their width.[16] Thus, we could join different sections of nanoribbons in order to construct a FET or a resistance.

In Fig. 1 we present the basic geometry of the proposed gate. It is made from three sections of armchair nanoribbons. The middle section is always chosen in such a way that the number of carbon atoms along the width (denoted by W_2) is of the form $3p$, where p is an integer. As a result, the central section exhibits an energy gap and is semiconductor.[16] This nanoribbon is connected with two nanoribbons chosen to have a more metallic character by adjusting W_1 in order to have $3p+1$ or $3p+2$ carbons atoms.[16] In fact, under a tight-binding approach, a nanoribbon with $3p+2$ carbons atoms has zero gap and is completely metallic. However, when first-principles calculations are made, there is also a small gap due to the edge effects.[16,17] Therefore, one expects a better performance of the device when using a $3p+2$ armchair ribbon for the noncentral sections. Experimentally, we propose that this central segment should be in contact with a plate, which could be fabricated by using high-resolution lithography. A potential could be applied to the substrate in order to control the performance.

Before doing any calculation, let us explain how the gate works. In Fig. 2 we show an schematic view of the band structure for the three sections of the gate. The middle section exhibits an energy gap, while the other sections are metallic. Due to the semiconductor nature of the central nanoribbon, the conductance is very small. However, when a potential is applied in the central section, the central band moves by a quantity eV, and the conductivity is increased since new states are available as the central conic band is displaced.

In order to test this intuitive idea, we have calculated the electrical conductivity by using the Kubo formula. Such calculation is made as follows. The electronic properties of graphene could be well described by a simple tight-binding Hamiltonian,[9]

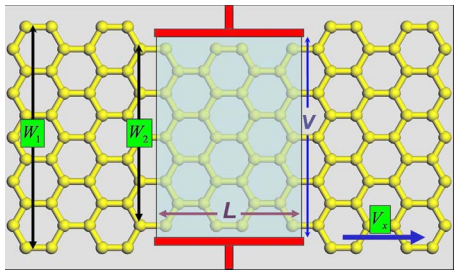

FIG. 1. (Color online) A gate of length L made from graphene nanoribbons of widths W_1 and W_2. An electric potential V is applied to control the gate. The current is produced by a potential V_x in the x direction.

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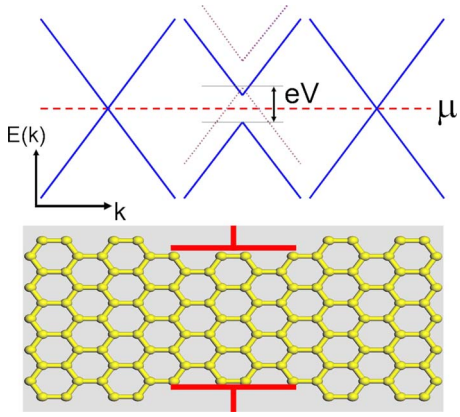

FIG. 2. (Color online) Schematic representation of the bands at each section. When the field is zero, the chemical potential μ at the central section falls in a gap. By applying an electric field eV, the central band is moved in such a way that μ falls in the band.

$$H = \sum_{j=1}^{N} \left(\varepsilon_0 |j\rangle\langle j| + \sum_{j \neq l}^{N} W(j,l)|j\rangle\langle l| \right), \tag{1}$$

where ε_0 is the self-energy of carbon atoms. $W(j,l)$ is the resonance integral which can be taken as a constant $\gamma_0 = 0.9$ eV for nearest neighbors and zero otherwise.[9] Using this Hamiltonian and the proposed geometry, it is possible to calculate the conductivity under the influence of an electrical field by using the Landauer formalism or the Kubo formula. Here we use the Kubo approach. This formula allows to calculate the a.c. electrical conductivity at frequency ω as follows:[18]

$$\sigma_{\alpha\nu}(\omega,T) = \frac{2e^2\hbar^2}{\pi\Omega m^2} \int_0^{\infty} dE \frac{f(E) + f(E+\omega)}{\hbar\omega} \times Tr[p^{\alpha} \operatorname{Im} G(E) p^{\nu} \operatorname{Im} G(E)], \tag{2}$$

where Ω is the system volume, α and ν are the Cartesian coordinates, $G(E) = \lim_{\eta \to 0}(E + i\eta - H)^{-1}$ is the Green function using a small imaginary part η, $f(E)$ the Fermi–Dirac distribution with chemical potential μ at temperature T,

$$f(E) = \frac{1}{\exp[(E-\mu)/k_B T] + 1}, \tag{3}$$

p^{α} is the projection of the momentum operator along the applied electric field given by

$$p^{\alpha} = \frac{iam}{\hbar} \sum_{j,l=1}^{N} [\mathbf{R}(j) - \mathbf{R}(l)]_{\alpha} W(j,l)|j\rangle\langle l|, \tag{4}$$

where $\mathbf{R}(j)$ is the position of particle j.

The d.c. electrical conductance, denoted by $\sigma_{\alpha\nu}(T)$, can be obtained form Eq. (2) in the limit $\omega \to 0$. It is noteworthy mentioning that for pure graphene, the Kubo formula produces a minimal conductivity different from zero, as observed experimentally.[8] However, the experimental and theoretical values differ by a small factor.[19] Furthermore, the Kubo formula produces different values depending on the order of the limits and damping due to impurities, and there have been plenty of discussions about the subject.[19] According to Ref. 19, the minimal conductivity for $\omega \to 0$ at nonzero temperature goes as $(\eta/8k_B T)$, measured in the natural units of conductance $\sigma_0 = e^2/h$. Thus, the minimal conductivity can vary over a wide range in units of σ_0 depending on η, which is a measure of the impurity scattering.[19] Here we are more interested in the relative conductance at different gate voltages and temperatures, and not in the absolute value of the minimal conductivity.

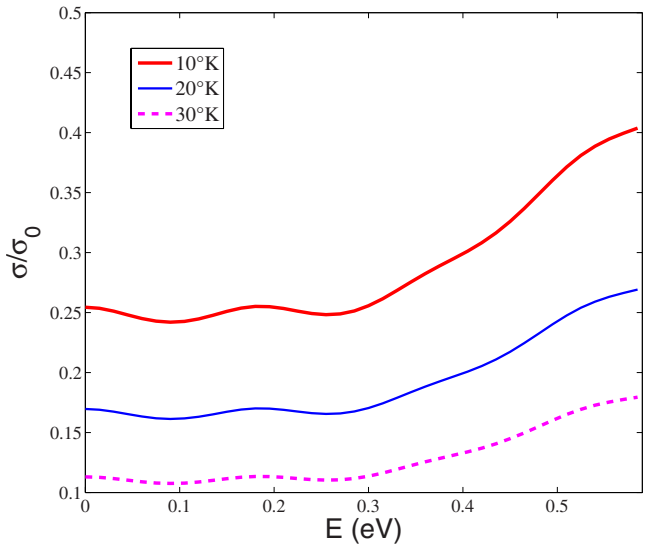

FIG. 3. (Color online) dc electrical conductivity of graphene as a function of gate voltage at low temperatures.

To compute the conductance we used infinite nanoribbons in the first and third sections. This was performed by matching the finite length transistor with the analytical solution obtained for an infinite metallic nanoribbon. A convenient way to compute the trace that appears in Eq. (2) is to diagonalize the matrix given by Eq. (1). If the resulting states are denoted by k, the eigenvalues by $E(k)$ and the resulting change of basis matrix transformation by U, and due to the invariance of the trace under unitary transformations, we obtain,

$$Tr[p^{\alpha} \operatorname{Im} G(E) p^{\nu} \operatorname{Im} G(E)] = Tr[p'^{\alpha} \operatorname{Im} G'(E) p'^{\nu} \operatorname{Im} G'(E)], \tag{5}$$

where $\operatorname{Im} G'(E)$ is now a diagonal operator given by

$$\operatorname{Im} G'(E) = \operatorname{Im} U^{-1} G U = \lim_{\eta \to 0} \sum_{k=1}^{N} \frac{\eta |k\rangle\langle k|}{[E - E(k)]^2 + \eta^2}, \tag{6}$$

and p'^{α} is

$$p'^{\alpha} = U^{-1} p^{\alpha} U = \frac{iam}{\hbar} \sum_{j,l=1}^{N} [\mathbf{R}(j) - \mathbf{R}(l)]_{\alpha} \times U^{-1}(k,j) W(j,l) U(l,k) |k\rangle\langle k|.$$

In Figs. 3 and 4 we present the behavior of the conductance at low and high temperatures. In both cases, we have assumed a worst case scenario, where a strong damping is present due to the corrugated nature of graphene sheets, phonon collisions, and interactions with the substrate. Such damping was included by using $\eta = 0.1$ in the Green function, which gives a good agreement with the experimental values found in pure graphene for the minimal metallic conductivity. For smaller dampings, some oscillations are observed in the conductance. The simulated gate was obtained using nanoribbons with nine carbon atoms in the middle section

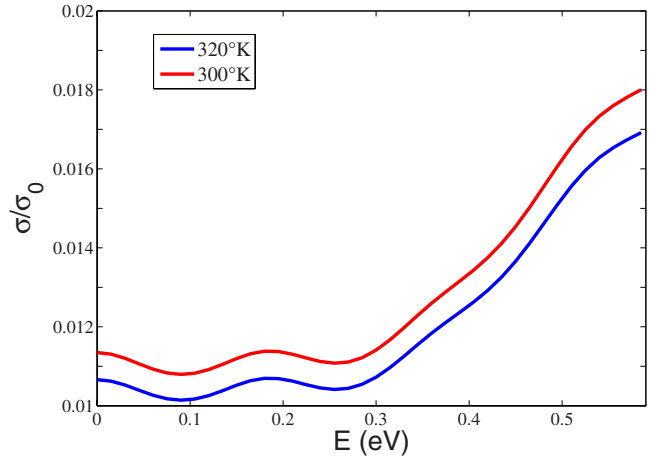

FIG. 4. (Color online) dc electrical conductivity of graphene as a function of gate voltage at high temperatures.

(p=3), and 11 in other sections. In Figs. 3 and 4, one can clearly see that once the gap is overcome the gate allows to flow a current, which is nearly 50% higher (for an energy of 0.5 V) than the current when the gate is closed.

The electronic transport could be tuned by changing the length of the central section, as shown in Fig. 5, where we show the conductance as a function of the gate voltage for three different central lengths N_L=8, 12 and 16. N_L denotes the number of atomic columns in the central section of the gate. From this figure, it is clear that an increase of the central section leads to a reduction in the conductance for low voltages, while the conductance is nearly similar when the control gate voltage is increased. Such behavior could be understood from the band structure presented in Fig. 2. If L is small, the probability for an electron to tunnel through the central barrier is higher, since such probability goes as $\sim e^{-kL}$. In fact, the presented device could also be used as a resistor when the central electrodes are removed. Different values of the resistance could be obtained by choosing the appropriate length L. In conclusion, we have presented a simple design to build a field effect gate and a resistance using graphene nanoribbons of different widths.

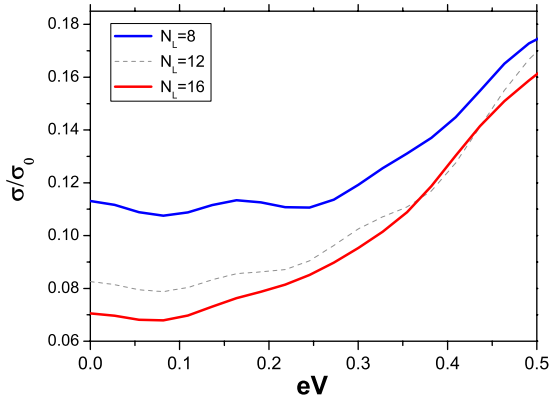

FIG. 5. (Color online) Conductance for three different lengths L of the central section at T=30 K. N_L is the number of vertical columns of atoms in the central section.

We thank FICSAC-UIA, DGAPA-UNAM Grant No. IN.115008; CONACyT Grant Nos. 48783-F, 50368, and 56787; Laboratory for Nanoscience and Nanotechnology Research-LINAN Grant No. 45772 (M.T.), Inter American Collaboration Grant No. 58899 (M.T.) and Grant No. 45762 (H.T.), Fondo Mixto de San Luis Potosí Grant No. 63001 S-3908 (M.T.), Fondo Mixto de San Luis Potosí Grant No. 63072 S-3909 (H.T.). We also thank Angélica L. Zamorategui for her assistance in running the programs. Calculations were carried at the KanBalam Supercomputer of UNAM.

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