Study of Carbon-Based Transistors with Semi-Analytic and Full-Band Models

Yi Zheng[1], Fernando Zanella[2], Guido Valerio[1], Cesar A. Dartora[2], and Zhuoxiang Ren[1]

[1]Sorbonne Universités, UPMC Univ. Paris 06, F-75005 Paris, France USA, yi.zheng@upmc.fr
[2]Electrical Engineering Department, Federal University of Paraná (UFPR), Brazil, fernando.zanella@gmail.com

In this work, the current-voltage characteristics of a double-gate graphene-based transistor are computed with different methods. A simplified semi-analytic method allows fast computation of the electric parameters by granting a good accuracy. A more complex method based on the solution of Schrodinger equation by means of non-equilibrium Green's function is used to validate the semi-analytic one. The codes will be used to evaluate the impact of mechanical stresses on this novel class of nano-transistors, where they are aimed for applications in the domain of flexible electronics.

***Index Terms*—Nanotransistors, graphene nanoribbon, deformation, non-equilibrium Green's function, flexible electronics.**

I. Introduction

Carbon-based nanotransistors have recently attracted a lot of attention due to their remarkable electronic properties [1]-[3]. As one of the emerging carbon materials, graphene has rapidly become an ideal candidate for flexible electronic devices [4]. In this connection, geometric deformation of graphene-based active components is an important issue.

In Fig.1 is shown a graphene nanoribbon in a field-effect transistor (FET). This geometric configuration will be considered in this paper. In our study, a strain is enforced on the FETs along the direction of the channel. A compact model in Section II will be compared and validated with a rigorous approach in Section III. The two models will be used in the final paper to study the impact of mechanical strains on the transistor properties.

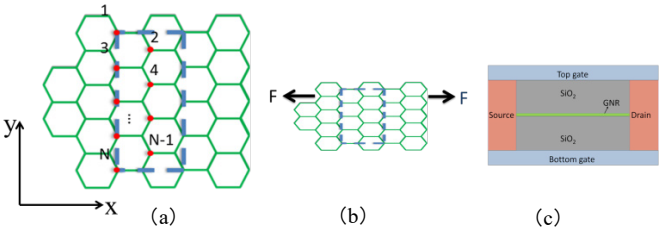

Figure 1. (a) Armchair graphene nanoribbon, (b) deformed graphene nanoribbon, (c) sectional view of a double-gate aGNR FET.

II. Compact Model

In this section, we propose a semi-analytical model for graphene based transistor. In the absence of any deformation, graphene energy bands can be calculated with tight binding model [5]. In the presence of a relative deformation d ($-0.1 \leq d \leq 0.1$), the hopping parameters change accordingly, thus determining a shift of Fermi points [6]. The energy bands of the graphene nanoribbon can be obtained:

$$E_\alpha^d(k) \cong \pm V\sqrt{1+4\cos\left[(1+d)\frac{\sqrt{3}ak}{2}\right]A_\alpha+4A_\alpha^2} \quad (1)$$

where

$$A_\alpha = \cos\left(\frac{\pi\alpha}{N+1}-\Delta k_y\right), \qquad \alpha = 1,\dots,N$$

$$\Delta k_y = -\frac{\sqrt{3}}{2}S_t(1+\nu)d \quad (2)$$

α=1,…, N defines the energy band, $a=\sqrt{3}a_{CC}$ and a_{CC} is the atomic distance between two adjacent atoms, V = 2.7 eV is the tight-binding hopping energy without deformation. S_t is a constant and ν is the Poisson's ratio of the graphene, usually taken approximately equal to 0.145.

Starting from (1), the effective mass, density of states and transmissivity coefficients T_s and T_d through the source and drain can be derived. These parameters are used to calculate the current by using the Landauer–Büttiker approach [7]:

$$I_i(\phi_c) = \frac{q}{\pi\hbar}\sum_\alpha \int_0^{E_\alpha^{\max}-E_\alpha^d(0)} \frac{T_sT_d}{T^*}[f_s-f_d]\mathrm{d}E \quad (4)$$

q being the electronic charge, f are Fermi-Dirac distributions of source and drain, respectively. The integration is performed over all the allowed energies in (1). The surface potential ϕ_c can be calculated by equating the microscopic charges $Q_{e/h}$ and the macroscopic charge Q_{macro}:

$$\frac{Q_{e/h}}{q} = \sum_\alpha \int_0^{E_\alpha^{\max}-E_\alpha^d(0)} D_\alpha(E)\left[\frac{T_s(2-T_d)}{T^*}f_s + \frac{T_d(2-T_s)}{T^*}f_d\right] \quad (5)$$

$$Q_{macro}[\varphi_c(x)] = -\sum_{i=g,s,d} C_i\left(V_i - V_{FB,i} - \varphi_c\right) \quad (6)$$

where C_g, C_s and C_d are the capacitances of gate, source and drain, V_g, V_s, V_d are the voltage of gate, source and drain, respectively, and $V_{FB,i}$ are the relevant flatband voltages.

III. Non Equilibrium Green's Function Method

The non-equilibrium Green's function (NEGF) method is a powerful tool to study transport phenomena in nanodevices. An extensive treatment of NEGF can be found in [8]-[9]; here we give a few definitions of NEGF as a statistical expectation

value between the product of fermions operators at different positions i and j, at different times t and t'. A full Green's function is given by

$$G_{ij}^{c} = -i\langle T\left[c_i(t)c_j^{\dagger}(t')\right]\rangle, \tag{7}$$

where $c_j^{\dagger}(t')$ creates one electron at site j at time t' and $c_i(t)$ annihilates an electron at site i at time t. T is a time-ordering operator that guarantees causality. As we are dealing with electrons, the c operators satisfy the anti-commutation relation $\{c_i, c_j\} = 0$, $\{c_i^{\dagger}, c_j^{\dagger}\} = 0$ and $\{c_i, c_j^{\dagger}\} = \delta_{ij}$, where $\{A, B\} = AB + BA$. (7) leads to the retarded Green's functions [10],

$$G_{ij}^{r}(t,t') = -i\theta(t-t')\langle\{c_i(t), c_j^{\dagger}(t')\}\rangle \tag{8}$$

where $\theta(t)$ is the Heaviside function. Since Fig. 1 ilustrates a 2D device, every atom can be indexed with a couple of integers. The interaction between sites should rather be described by the indexes mn, ij. To apply (8) to the nanoribbon in Fig. 1a, the equation of motion must be enforced:

$$i\partial_t G_{mn,ij}^{r}(t,t') = (t-t')\delta_{mn,ij} - i\theta(t-t')\langle\{[c_{mn}, H], c_{ij}^{\dagger}\}\rangle. \tag{9}$$

The comutator in the second term of (9) comes form the Heisemberg expression for the time evolution of c

$$i\frac{dc_{mn}}{dt} = [c_{mn}, H], \tag{10}$$

where the reduced Planck constant is set to unity ($\hbar = 1$) by suitably scaling the Hamiltonian H. All the physics will be described by the Hamiltonian in (9), including electron-electron interactions H_{ee}, phonons and photons interactions H_{ph}, or even electromagnetic interactions H_{EM}:

$$H = \sum_l \mu c_l^{\dagger} c_l + \sum_l V c_{l+1}^{\dagger} c_l + H_{ph} + H_{EM} + H_{ee}. \tag{11}$$

In (11) μ is the energy of each site (red dots in Fig. 1), V is the hopping energy. l is the double-index m. If the interaction is a simple external bias, to simulate the device in Fig.1c, the H_{EM} term is given by the solution to the Poisson's equation with proper boundary conditions.

By Fourier transforming (9) we obtain

$$(\omega - \sum_{mn}\delta_{ij,mn}q\varphi)G_{ij}^{r}(\omega) = \delta_{ij,mn} + \sum_{mn} V G_{ij,mn}^{r}(\omega), \tag{12}$$

where $\mu = 0$, ω is an energy parameter. (12) has a matrix form and is iterative, which means that it can be applied to a real device by considering it as composed by several adjacent layers of atoms (each layer being a vertical line of connected atoms in Fig. 1a). By applying (12) to the FET of Fig. 1 is possible to deduce that current is given by

$$I_{ds} = \frac{2q}{\hbar}\int d\omega[G_{l1}\Gamma_{11}G_{l1}^{a}(f_s(\omega-\varphi_s) - f_d(\omega-\varphi_d)) - S(\omega)]$$

$$S(\omega) = iG_{ll}f_d(\omega-\varphi_d), \tag{13}.$$

IV. Numerical Results

In Fig. 2 we show the current I_{ds} computed by means of the compact model described in Section II and the NEGF method of Section III. The current is shown for different values of drain-source voltage V_{ds} by keeping a zero gate voltage $V_g = 0$ V. For simplicity, the current has been computed in the absence of a dielectric between the gates, even if both the methods can deal with the presence of a dielectric. As shown in the figure, the very good agreement between the methods fully validates the simplified approach. These results are obtained in the absence of deformation; however, in the final paper the effect of deformation will be included in both methods and a full discussion on both physical and computational aspects will be given.

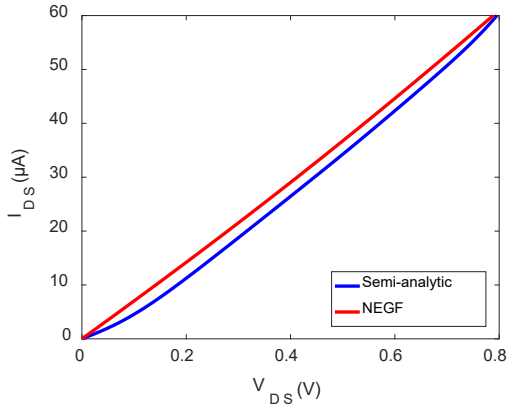

Figure 2. Current I_{ds} vs. drain-source voltage V_{ds}. $V_g = 0$ V, no dielectric is present between the gates.

V. Conclusion

A simple compact model has been compared with an accurate method based on NEGF, yielding very good agreement. At the conference, a full validation will be presented on the impact of mechanical stress on transistors.

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