



Carbon – Science and Technology

ISSN 0974 – 0546

<http://www.applied-science-innovations.com>

Received : 12/11/2012, Accepted : 15/11/2012

Advanced Modeling of the Electrostatic Field Coupling in Graphene Nanoribbons

Luca Pierantoni ^(A, B)

(A) Dipartimento di Ingegneria dell'Informazione, Università Politecnica delle Marche, Via Brecce Bianche 12, 60131, Ancona, Italy.

(B) Italian Institute of Nuclear Physics (INFN) - Laboratori Nazionali di Frascati, via Enrico Fermi 40, Frascati (Roma), Italy.

The field coupling of Graphene NanoRibbons (GNR), which is very important from the view point of realistic configurations / applications such as in field effect transistor, interconnects, plasmonic transmission lines, is analyzed and presented in this communication. We consider the quasi-static response of two GNRs coupled by Coulomb interaction : the Schrödinger equation in the two dimensional (2D) domain of the GNRs is solved together with the three dimensional (3D) Poisson equation. It is observed that, unless the two GNRs are very close to each other, their Coulomb interaction is not so strong, in the sense that their charge and potential distributions are just slightly distorted by the presence of the other GNR. The effect is even lower in the case of semimetallic GNRs, where the modulation of current and charge by external potential is known to be intrinsically small, owing to the absence of an energy band gap.

Introduction : Radio-frequency (RF) nanoelectronics represents an emerging branch of nanotechnology with possibilities for unprecedented microwave, millimeter-wave and THz devices and systems [1, 2]. It is remarkable to note that many nano-scale materials and devices (e.g. carbon-based), exhibit their most interesting properties over a broad range of applications and operating frequencies, covering the radiofrequency (RF) spectrum, through the microwave up to the optical region. Among these novel materials, graphene, made of carbon atoms packed in a two dimensional (2D)-honeycomb lattice, is quickly becoming an extremely interesting option for a wide variety of electronic devices and circuits, from field effect transistors (FET), interconnects to low-noise amplifiers and nonlinear electronics. It offers the possibility of outstanding performances with much lower power draw, using processing technology compatible to that used in advanced silicon device fabrication (CMOS).

The analysis of GNRs can be carried out by discrete models such as tight binding (TB), and continuous models, such as effective mass and $k\cdot p$ approximations, which stems from the approximation of TB around particular points of the dispersion curves. The $k\cdot p$ model leads, for the GNR, to a Dirac-like system of equations [3]. Another popular approach for the calculation of quantum transport is given by the use of the Green's function of a GNR region [4 - 6]. This method is closely related to the approach reported in [7], which breaks up the system into layers perpendicular to the transport direction. All techniques mentioned above are demonstrated to be as, for example, the effects on charge transport of applied external electric and magnetic fields, bending, lattice defects and discontinuities, edge terminations and so on.

However, the latter methods requires high computational resources, and can hardly include the effect of i) The self-generated electromagnetic

(EM) field, ii) impinging external EM fields. Recently, we have introduced full-wave techniques both in the frequency (energy)-domain [8 - 11], and the time-domain [12 - 15] for the investigation of new devices based on carbon materials, namely carbon nanotube (CNT), multiwall (MW) CNT, graphene, and GNR.

In both the approaches, the quantum transport is described by the Schrödinger equation or its Dirac-like counterpart. The electromagnetic field provides sources terms for the quantum transport equations, that, in turns, provides charges and currents for the electromagnetic field.

In the present work, we investigate the quasi-static response of two GNRs coupled by Coulomb interaction by means of an effective Scattering Matrix approach [8 - 11]. This problem has a remarkable impact in fabricated devices, as the amount of the field coupling may strongly affect the performances of, e.g. GNR-based field effect transistor, interconnects, plasmonic transmission lines.

The Schrödinger equation, describing the coherent charge transport in the 2D GNR-domain, is solved together with the Poisson equation in the whole three dimensional domain. We observe that, unless the two GNRs are very close to each other, their Coulomb interaction is weak and their charge and potential distributions are just slightly distorted as compared to the case of isolated GNRs. This is particularly true of the case of semimetallic GNRs, where the absence of an energy band gap implies a small reaction of the charge spatial-density to local potential changes.

Modeling of Graphene Nanoribbons : The present model assumes not only that the e.m. wavelength is small as compared to the charge spatial variation, but also that the frequency of the electromagnetic (e.m.) field is very small as compared to the time dynamic, i.e. the energy, of the travelling particles. This kind of analysis can be applied in order to explore the basic working principles of graphene in its use as interconnect and as channel for field effect transistor (FET). For instance, a lumped-circuit model with parasitic capacitances, including the quantum capacitance of the graphene channel, can be easily

derived from the simulation results. This leads to a rough estimation of the gain and the unit-gain frequency. In practice, non-ballistic effects reduce the conductance of the interconnect, and the unit-gain frequency of the transistor.

The main result of the present work resides in that it shows, by means of some new examples, the effectiveness of the scattering-matrix approach for the solution of relatively large graphene systems involving thousands carbon atoms and consequent multichannel transport.

As already mentioned, the examples involve the coupling, through coulomb interaction, of two GNR channels, both semiconducting or both semimetallic, in a single FET transistor configuration. Differently from simulations performed at the atomic scale, that can deal very hardly with large carbon devices, we consider structures made of many thousands carbon atoms. Other common approaches that, similarly to ours, avoid *ab initio* calculation, like Non Equilibrium Green's Function (NEGF), could be successfully applied. The NEGF describes the carrier interaction through a spatial charge density that locally perturbs the graphene neutrality. The scattering matrix approach is equivalent to the NEGF, but, in our opinion, it better highlights the physical behavior of the system, because: i) It makes use of electronic modes that are easily normalized with respect to the physical current, ii) It considers the physical ports of graphene circuits by the same standard as the virtual ports, i.e. all the accessible electronic wavefunctions, iii) It treats all the ports as adapted ones, i.e. transparent or perfect absorbing, iv) It allows an easy check of the losslessness and reciprocity constraints involved in charge transport, through the scattering matrix properties, v) It allows the use of concepts well known in the microwave and RF community, such as cascade of transmission lines, transformers, lumped circuit elements, etc., all useful in order to model long graphene structures eventually containing defect, bending, discontinuities, and electrostatic perturbations.

An important parameter for the operation of a FET transistor is given by the gate differential capacitance: this parameter directly affects the frequency characteristics of the transistor, as the

unit gain frequency. The derivative, with respect to the gate bias, of the charge density in the channel, after self-consistent solution of the transport/electrostatic problem, provides the channel contribution to the gate capacitance. Some simple models, based on geometric and dielectric characteristics of the gate and the channel, may provide some partial results, by employing a metallic approximation for the channel. However, it is well known that the electromagnetic screening is much less effective in two dimensions than in three dimensions, and graphene behaves, to some extent, as an ideal two-dimensional electron gas. Hence, a rigorous analysis must include the knowledge of the actual electronic structure of the GNR channel, and its change under external voltage. The result is what usually is referred to as quantum capacitance, that is, the change of the channel energy-levels, and of the corresponding wavefunction distributions, due to an external applied voltage.

The Dirac equation is formulated in a discrete version [9] :

$$H_l \psi_l + H_0 \psi + H_r \psi_r = E \psi \quad (1)$$

where E is the energy, ψ_l, ψ, ψ_r are the wavefunctions of three consecutive GNR unit cells and the Hamiltonian has been decomposed in three matrices which model transfer energies between adjacent cells: matrix H_l (H_r) includes the hopping elements from a unit cell to the previous (following) one, H_0 is the self energy matrix of the unit cell. The relations $H_l = H_r^\dagger$ and $H_0 = H_0^\dagger$ hold. The diagonal elements of H_0 contain the electrostatic potential solution of the Poisson's equation. Exploiting the lattice periodicity, we have :

$$\begin{aligned} (H_l e^{jkL} + H_0 + H_r e^{-jkL}) \psi &= E \psi \\ \psi &= e^{-jk_y} \sum_i \psi_i \delta(x - x_i, y - y_i) \end{aligned} \quad (2)$$

where i spans the atomic sites, k is the wavenumber and L is the length of the unit cell. The solutions of equation (2), corresponding to different branches of the dispersion curves, can be distinguished as propagating modes for real k , and evanescent modes for complex or imaginary k . In

order to provide the correct mode normalization, wavefunctions have to be divided by :

$$A = \sqrt{\frac{f_T(E)}{4\pi \text{Im}(\psi^\dagger H_r e^{-jkL} \psi)}} \quad (3)$$

where f_T is the Fermi distribution function at T temperature ($T \sim 0$ has been used). The above normalization implies that all propagating modes carry the same current with reference to the Landauer's formula.

The scattering matrix \mathbf{S} of a GNR device, defined as in [21] relates incident and reflected mode amplitudes at port sections, which are different terminations of a many-lead GNR circuit.

One of the difficulties of the proposed method resides in that the scattering formulation has to be adapted to a periodic waveguide, where the right basis to be used for describing charge transport is given by the complete set of Floquet, or periodic, modes. Within the latter choice the scattering parameters can be shown to obey, for example, the expected reciprocity and losslessness constraints, respectively $\mathbf{S} = \mathbf{S}^T$ and $\mathbf{S}^\dagger \mathbf{S} = \mathbf{I}$.

The number of modes at any port depends on the port size, on the Fermi level, and on GNR chirality. Regressive modes, either above or below cut-off, are scattered out of the GNR without reflection: this means perfectly transparent ports.

In case of a two-port GNR, the charge density is obtained by summing the normalized wavefunctions of carriers injected from the two opposite ports :

$$Q = -e \sum_i \int \left\{ f_1(E) \frac{|\psi_1^i(x, y, E)|^2}{A^2} + f_2(E) \frac{|\psi_2^i(x, y, E)|^2}{A^2} \right\} dE \quad (4)$$

where the upper index “ i ” of $\psi_{1,2}^i$ indicates the i -th band whereas the lower ones indicate the ports, f_1 and f_2 are the Fermi probabilities for the electrons at ports 1 and 2 respectively, $e = 1.6 \cdot 10^{-19}$ C. The charge density (4) is assumed as source term in the familiar Poisson equation for the potential V .

For a multiport device all physical quantities are obtained by including the charge contributions from all ports. For instance, the total current flowing through the p -th port includes contribution of all modes transmitted from the port p to all the other ports :

$$I_p = \frac{2e}{h} \sum_{i,j,q} \int (f_p(E) - f_q(E)) S_{pq}^{i,j}(E) dE \quad (5)$$

where $S_{pq}^{i,j}$ is the scattering coefficient from mode i to mode j , and from port p to port q .

Results : As described in [8-10], we solve the coupled Poisson-Dirac system of equations :

$$\nabla^2 V = \frac{\rho_T}{\epsilon} \quad \rho_T = q \int |\psi(\mathbf{r}, E)|^2 dE \quad (6)$$

$$\underline{H}\Psi = v_F \sigma \mathbf{k} = E \Psi(\mathbf{r}, t) \quad (7)$$

The Poisson equation (6), is solved by an appropriate FDFD scheme. It has to noted that, in the iterative process, from the wavefunctions Ψ , solution of the Dirac equation (7), the charge density ρ_T , is derived. This charge density is the source term for a new a new potential distribution $V(\rho_T)$, that, in turns, is inserted into the Hamiltonian of the Dirac equation. Boundary condition for the Poisson equation include metal contacts, dielectric materials, bias, etc., and any kind of initial quantum potential profile. The numerical convergence of the iterative approach is achieved when the surface integral of the absolute value of the difference between the potential V distribution at the $(n-1)^{th}$ and n^{th} iteration is below the numerical machine accuracy.

We analyze the potential (electric field) distribution in a region occupied by two laterally coupled GNR, that is very challenging problem, e.g. in the case of GNRs array in a FET configuration, Figure (1), or using GNRs as interconnects, Figure (2). The coupling takes place by means of the Coulomb interaction. In particular, we focus on the FET configuration: two semiconducting GNRs connect source and drain of a FET-like device. A potential difference of 0.1 V is applied between drain and source; the source is assumed at 0 V, equipotential with the

lateral gate (G). The GNRs are about 2.2 nm wide and the area of the square “window” delimited by the electrodes is 20x20 nm².

We make the hypotheses of a metal-to-GNR doping by assuming a 2.9 eV shift of the Dirac point, in order to place the Fermi level about 0.7 eV above the band gap. In this case, we have appreciable charge injection from the metal to nanoribbon “bridges”. In practice, a smaller doping still can imply a strong effect when wider GNR, i.e. smaller band gaps, are considered. It is noted that the self-consistent potential of Figure (3b), with $d=0.15$ nm, is strongly different from the potential of Figure (3a), with $d=2.4$ nm. As largely expected, changing the distance between the GNR does not simply imply a potential “composition” following a superposition of effects : the iterative process develops very differently in the two cases, and the final results are not easily predictable.

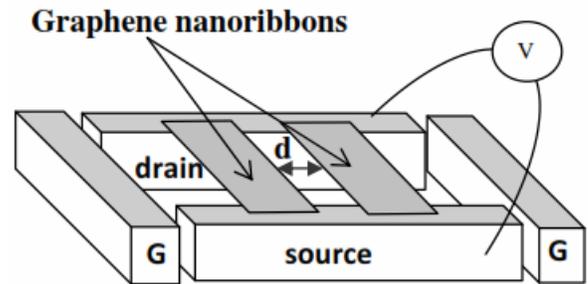


Figure (1) : Graphene nanoribbon in a FET configuration.

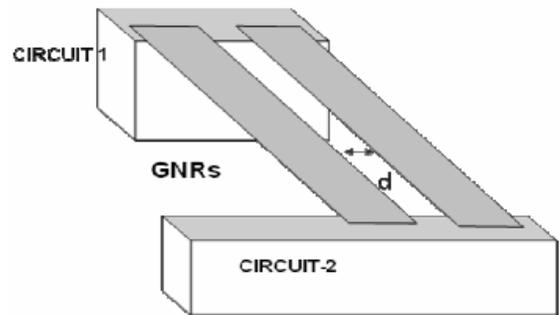


Figure (2) : Graphene nanoribbons as circuit interconnections.

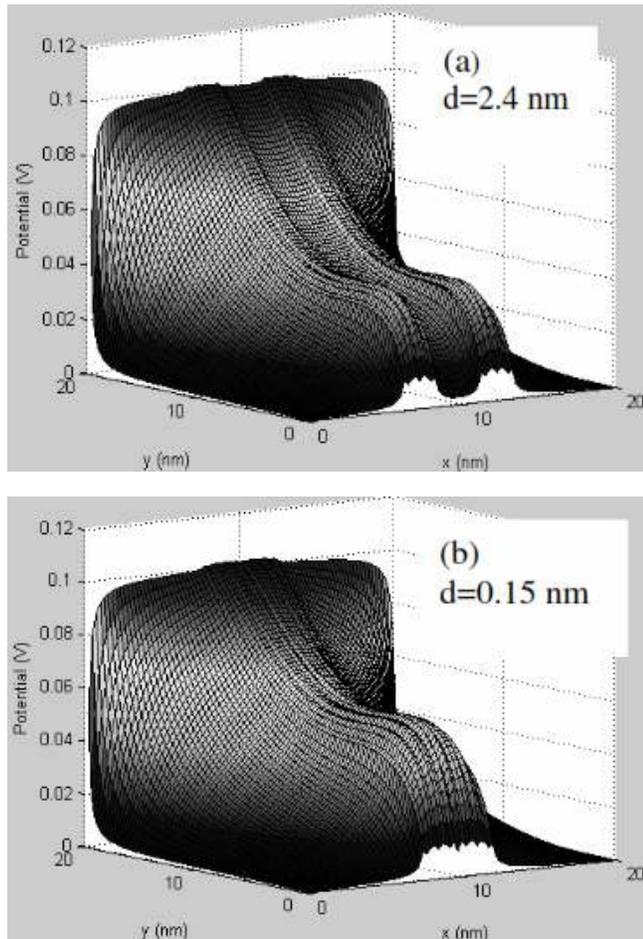


Figure (3) : Potential (electric-field) distribution in terms of the distance d between the two GNRs. (a) $d=2.4$ nm and (b), $d=0.15$ nm.

Conclusions : I report on the investigation of field coupling of nanoribbons (GNR), a truly challenging problem in fabricated devices, as the amount of the cross-talk field coupling may strongly affect the performances of, e.g. GNR-based field effect transistor, interconnects, plasmonic transmission lines.

I analyzed the quasi-static response of two GNRs coupled by Coulomb interaction: the Schrödinger equation in the 2D domain of the GNRs is solved together with the 3D Poisson equation.

The effect of changing the distance between the two GNR channels cannot be accounted by simply following the rule of superposition of the effects : the iterative nonlinear PS solution develops very differently for different distance, and the final results are not easily predictable. However, at least for low external voltages, the interaction is

generally weak, as the charge density in the channel is small. The interaction in the case of semimetallic GNRs is even weaker than in the case of semiconducting GNRs, as a result of the absence of bandgap.

References :

- [1] L. Pierantoni, "RF Nanotechnology - Concept, Birth, Mission and Perspectives", *IEEE Microwave Magazine*, vol. 11, no. 4, pp. 130-137, June 2010.
- [2] L. Pierantoni, F. Coccetti, P. Lugli, S. Goodnick, "Guest Editorial", *IEEE Transactions on Microwave Theory and Techniques*, vol. 59, no.10, Oct. 2011, pp. 2566-2567.
- [3] L. Brey and H. A. "Electronic States of Graphene Nanoribbons Fertig", *Cond-matt*. 0603107, 5 Mar 2006.
- [4] S. Raulot, "Green functions for the Dirac operator under local boundary conditions and applications", *Cond-mat*, 0703197, 2007.
- [5] Y. Yoon, G. Fiori, S. Hong, G. Iannacone, J. Guo, "Performance Comparison of Graphene Nanoribbon FETs With Schottky Contacts and Doped Reservoirs", *IEEE transactions on electron devices*, vol. 55/9, pp 2314, 2008.
- [6] Z. F. Wang, R. Xiang, Q. W. Shi, J. Yang, X. Wang, J. G. Hou and J. Chen, "Modeling STM images in graphene using the effective-mass approximation", *Physical Review B* 74, 125417, 2006.
- [7] D. Mencarelli, T. Rozzi, C. Camilloni, L. Maccari, A. di Donato, L. Pierantoni, Modeling of Multi-wall CNT Devices by Self-consistent Analysis of Multi-channel Transport, *IOP Science Nanotechnology*, vol. 19, Number 16, April 2008.
- [8] D. Mencarelli, T. Rozzi, L. Pierantoni, "Coherent Carrier Transport and Scattering by Lattice Defects in Single- and Multi-Branch Carbon Nanoribbons", *Physical Review B*, vol.77, pp.1954351-11, May 2008
- [9] D. Mencarelli, T. Rozzi and L. Pierantoni, Scattering matrix approach to multichannel transport in many lead graphene nanoribbons, *IOP Science, Nanotechnology*, vol. 21, no.15, 155701, pp. 1-10, March 2010.
- [10] D. Mencarelli, L. Pierantoni, M. Farina, A. Di Donato, T. Rozzi, A multi-channel model for the self-consistent analysis of coherent transport in graphene nanoribbons, *ACS Nano*, Volume 5, Issue 8, 23 August 2011. pp. 6109-6128.
- [11] G. Vincenzi, G. Deligeorgis, F. Coccetti, M. Dragoman, L. Pierantoni, D. Mencarelli, R. Plana, Extending ballistic graphene FET lumped element models to diffusive devices, *Solid-State Electronics*, vol. 76, Oct. 2012, pp. 8–12.
- [12] L. Pierantoni, D. Mencarelli, and T. Rozzi, "Boundary Imittance Operators for the Schrödinger-Maxwell Problem of Carrier Dynamics in Nanodevices", *IEEE Trans. Microw. Theory Tech.*, vol. 57, issue 5, pp. 1147-1155, May 2009.
- [13] D. Mencarelli, L. Pierantoni T. Rozzi, Graphene Modeling by TLM approach, *Microwave Symposium Digest, 2012 Int. Microwave Symposium, Montreal, QC, Canada*, June 17-22, 2012, pp. 1-3.
- [14] L. Pierantoni D. Mencarelli, T. Rozzi, Advanced Techniques for the Investigation of the Combined Electromagnetic-Quantum Transport Phenomena in Carbon Nanodevices, *Proc. of the Int. Conference on Electromagnetics in Advanced Applications (ICEAA) 2012-IEEE APWC 2012-EEIS 2012*, Cape Town, South Africa, Sept. 2-7, 2012, pp. 873–876.
- [15] L. Pierantoni, A. Massaro, T. Rozzi, Accurate Modeling of TE/TM Propagation and Losses of Integrated Optical Polarizer, *IEEE Trans. Microw. Theory Tech.*, vol. 53, no.6, June 2005, pp. 1856-1862.