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Gianluca Fiori and Giuseppe Iannaccone

***Abstract*—We present an atomistic 3-D simulation of graphene nanoribbon field-effect transistors (GNR-FETs), based on the self-consistent solution of the 3-D Poisson and Schrödinger equations with open boundary conditions within the nonequilibrium Green's function formalism and a tight-binding Hamiltonian. With respect to carbon nanotube FETs, GNR-FETs exhibit comparable performance, reduced sensitivity to the variability of channel chirality, and similar leakage problems due to band-to-band tunneling. Acceptable transistor performance requires prohibitive effective nanoribbon width of 1–2 nm and atomistic precision that could in principle be obtained with periodic etch patterns or stress patterns.**

***Index Terms*—Atomistic tight-binding Hamiltonian, graphene, nanoribbon, nonequilibrium Green's function formalism (NEGF), 3-D Poisson.**

I. Introduction

In THE last decade, carbon nanotubes (CNT) have attracted extraordinary interest for their extremely interesting physical and electrical properties [1] and their potential as an alternative to silicon as channel material for transistors beyond complimentary metal–oxide–semiconductor technology [2]. Recent experiments by Novoselov *et al.* [3] demonstrated the possibility of fabricating stable single atomic layer graphene sheets, with remarkable electrical properties, that have brought new excitation to the field of carbon electronics.

Two-dimensional graphene is a zero-gap material, which makes it not suitable for transistor applications.

Energy gap can however be induced by means of lateral confinement [4], realized for example by lithography definition of narrow graphene stripes, i.e., the so-called graphene nanoribbons.

Experiments on graphene-based devices [5] and graphene nanoribbon field-effect transistors [6] (GNR-FETs) have appeared only very recently and demonstrate limited capability to modulate the conductance of a graphene channel at room temperature. The main problem is the need to fabricate extremely narrow nanowires (on the order of 1 nm) with atomic precision to obtain an energy gap adequate for room temperature operation.

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Since at the moment the fabrication technology is at its very first steps, computer simulations can be very useful to provide physical insights of GNR-FETs and to estimate the attainable performance. Recent theoretical works have shown that graphene nanoribbons have an energy gap that has an oscillating behavior as a function of width, with average roughly proportional to the inverse width, and that edge states play a very important role in inhibiting the existence of fully metallic nanoribbons [7]. Such behavior cannot be reproduced if one does not consider edge effects [8].

Likewise, from the simulation point of view, research on GNR-FETs is at an embryonic stage: the only works available in the literature [9], [10] are based on a semiclassical analytical top-of-the-barrier model. For short-channel transistors, only a 3-D simulation is suitable for an accurate evaluation of the electrostatics and of intraband and interband tunneling.

To this purpose, we have developed a code for the simulation of GNR-FETs, based on the nonequilibrium Green's function formalism (NEGF), with a tight-binding Hamiltonian built from a p_z orbital basis set in the real space, which has been included in our in-house 3-D device simulator NANOTCAD ViDES [11]. We will show that GNR-FETs have performance comparable with CNT-FETs and that can be greatly affected by the channel width and edge roughness.

II. Physical Model and Results

Our approach is based on the self-consistent solution of the 3-D Poisson and Schrödinger equations with open boundary conditions [12], which is able to take into account fully ballistic transport, in order to outline the higher limits of device performance, as well as elastic scattering due to line edge roughness. The Hamiltonian is taken from [7], in which edge states at the nanoribbon lateral ends have been considered. In this letter, we refer to $(N, 0)$ armchair graphene nanoribbons, which consist of an unrolled $(n, 0)$ zigzag nanotube with $N = 2n$.

The considered double-gate GNR-FETs have the structure depicted in the inset of Fig. 1. The gates are metallic, the oxide thickness t_{ox} is equal to 1 nm, the channel is 15 nm long, and W is the channel width. The source and drain extensions are 10 nm long and are doped with a molar fraction of fully ionized donors $f = 5 \times 10^{-3}$. The spacing between parallel GNRs is 4 nm.

In Fig. 1, the transfer characteristics of a (12,0) GNR-FET ($W = 1.37$ nm) for drain-to-source voltage V_{DS} of 0.1 and 0.5 V are shown and compared to those of a (16,0) CNT-FET with the same geometry (same t_{ox}, L, and device spacing), whose energy gap E_{gap} is close to that of the GNR-FET and equal to 0.6 eV.

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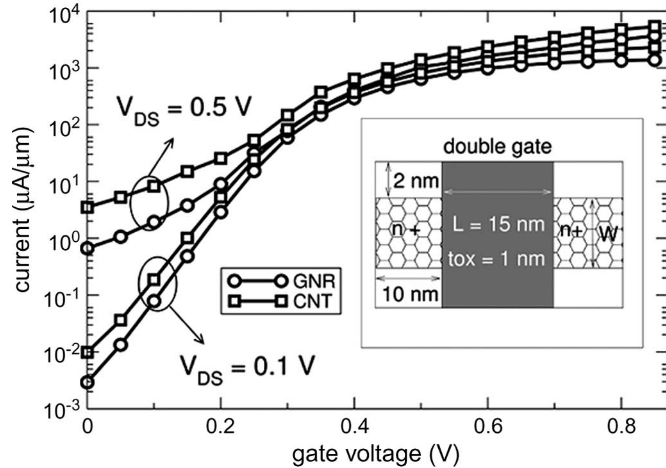

Fig. 1. Transfer characteristics of double-gate CNT and GNR-FETs, with doped source and drain reservoirs, with channel length equal to 15 nm, oxide thickness t_{ox} equal to 1 nm, and channel width $W = 1.37$ nm. The lateral space is equal to 2 nm. Inset: Sketch of the GNR-FET.

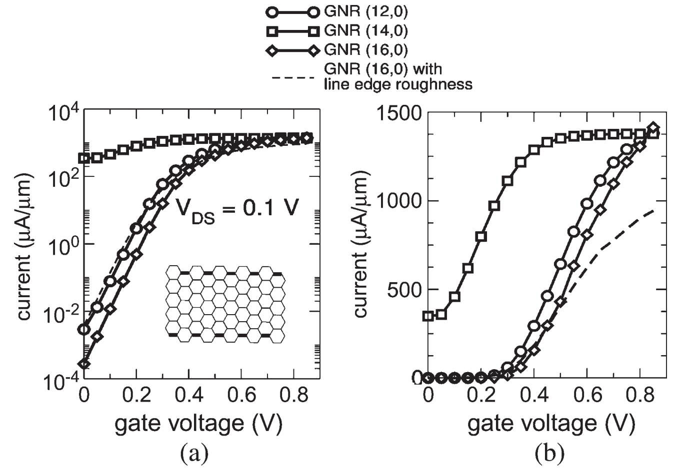

Fig. 2. Transfer characteristics in the (a) logarithmic and sensitivity on (b) linear scale of GNR-FETs with different chiralities: (12,0), (14,0), and (16,0) (channel width W equal to 1.37, 1.62, and 1.87 nm, respectively), for $V_{\mathrm{DS}} = 0.1$ V. (Dashed line) Transfer characteristic for the (16,0) GNR-FET when roughness at the lateral edge of the GNR is considered. Inset: Sketch of the graphene nanoribbon, where randomly decoupled atoms have been highlighted by thick lines.

Good control of the channel by the gate potential is shown at $V_{\mathrm{DS}} = 0.1$ V, since the subthreshold swing S for the GNR-FET and the CNT-FET are 64 and 68 mV/dec, respectively. For $V_{\mathrm{DS}} = 0.5$ V, we observe a pronounced degradation of S, with $S = 191$ mV/dec for the GNR-FET and almost 250 mV/dec for the CNT-FET. This has to be imputed to hole-induced barrier lowering (HIBL) [12]: in the subthreshold regime, when sufficiently high V_{DS} is applied, confined states in the valence band of the channel align with the occupied states in the drain, leading to band-to-band injection of holes in the channel.

If only elastic band-to-band tunneling can occur (as assumed in our simulation), the excess of holes in the channel lowers the channel potential, increasing the OFF current and S, as shown in Fig. 1: the lower the energy gap and the higher the V_{DS}, the higher the HIBL effect. HIBL is more pronounced in CNT-FETs than in GNR-FETs, because the conduction band of CNTs is double degenerated and therefore CNTs have twice the density of states of GNRs with the same gap.

If, on the other hand, inelastic band-to-band tunneling or Schockley–Read–Hall mechanisms are relevant, holes can recombine with electrons at the source and, instead of HIBL, we observe a leakage current from source to drain due to gate-induced drain leakage (GIDL) [13].

In strong inversion, the transconductance g_m at $V_{\mathrm{DS}} = 0.1$ V is 3600 and 6100 μS/μm for the GNR-FET and the CNT-FET, respectively, whereas at $V_{\mathrm{DS}} = 0.5$ V, we obtain $g_m = 4800$ μS/μm for the GNR and a $g_m = 8760$ μS/μm for the CNT. The advantage of CNT-FETs is due to the double degeneracy of the conduction band in CNTs.

It is known that a variability of the chirality of fabricated CNTs yields metallic nanotubes useless for transistor applications. For GNRs, this problem is mitigated, since all GNRs are semiconducting. In order to investigate quantitatively the effect of a finite fabrication tolerance on the width of GNRs, we have computed the transfer characteristics of GNR-FETs with different chiralities: (12,0), (14,0), and (16,0).

As can be seen in Fig. 2(a), the three devices behave as transistors but show very different behavior, even if they differ by only one carbon atom along the channel width. The problem is that the gap is still largely dependent on the chirality: the (16,0) GNR ($W = 1.87$ nm) has the largest gap ($E_{\mathrm{gap}} = 0.71$ eV), whereas the (14,0) ($W = 1.62$ nm) has the smallest gap ($E_{\mathrm{gap}} = 0.13$ eV). As a consequence, the (16,0) device shows the best gate control over the channel potential, whereas the (14,0) shows the worst: the energy gap is so small that elastic band-to-band tunneling occurs at the source and current is dominated by GIDL.

Such problem is reduced if rough edges are considered. We have considered the impact of line edge roughness in a (16,0) GNR-FET device, by randomly decoupling carbon atoms on the lateral boundaries of the GNR. The transfer characteristic for one example is shown in Fig. 2 (dashed line). Since the channel consists of several hundreds of rings, the rough GNR behaves as a GNR with an intermediate effective gap. More statistical simulations would be needed to assess the dispersion of the electrical characteristics, although the typical GNRs are probably long enough to provide sufficient averaging to suppress interdevice dispersion. Rough edge scattering strongly affects the ON current and the transconductance suppressing it by about 30% with respect to fully ballistic transistors. Additional suppression in realistic GNR-FETs can be due to defects, ionized impurities, and phonon scattering.

From the aforementioned simulations, it is clear that lateral confinement way beyond state-of-the-art etching capabilities would be needed to obtain adequate E_{gap}. We also found that electrostatic periodic potential modulation with a peak-to-peak value of a few volts is not sufficient to induce the required gap of a few hundred millivolts.

In order to evaluate whether a periodic strain pattern can allow to engineer the GNR gap, we have computed the energy gap in a (24,0) GNR ($W = 5.86$ nm), multiplying the overlap integral of the element of the Hamiltonian in correspondence to the couple of atoms in the middle of the GNR by a "strain factor" $\sigma : \sigma$ is larger than 1 for compressive strain, and

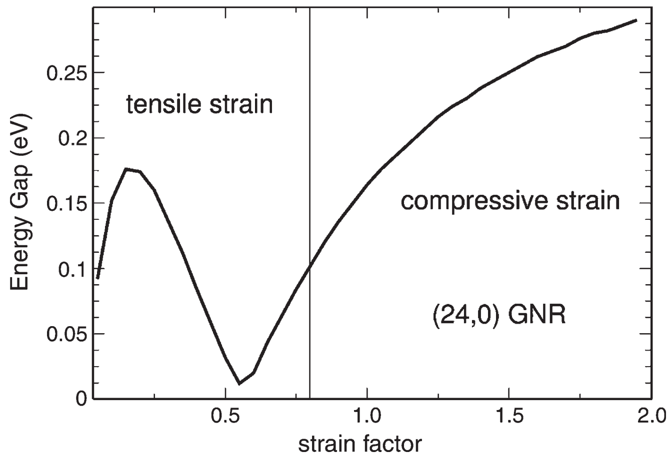

Fig. 3. Energy gap of a (24,0) GNR, when tensile and compressive strains are considered in correspondence to the middle of the nanoribbon, as a function of the strain factor by which the Hamiltonian elements of the strained carbon atoms are multiplied.

smaller than 1 for tensile strain. As can be seen in Fig. 3, compressive strain seems to be able to increase the energy gap of the nanowire by a significant amount. Of course, we can only suggest to experimentalists to evaluate the option.

III. Conclusion

In this letter, a simulation study of GNR-FETs has been performed by means of the self-consistent solution of the 3-D Poisson and Schrödinger equations with open boundary conditions within the NEGF formalism. Edge states have been considered at the lateral ends of the nanoribbon using the model proposed in [7]. GNR-FETs exhibit performance similar to CNT-FETs, also showing significant band-to-band tunneling when small gap devices are considered and large V_{DS} is applied. GNR-FETs are more robust than CNT-FETs with respect to variability of the channel chirality, and edge roughness seems to play a useful averaging effect. Finally, we suggest that periodic strain could in principle represent an alternative to etching for inducing an energy gap in graphene.

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References

[1] A. Javey, J. Guo, Q. Wang, M. Lundstrom, and H. Dai, "Ballistic carbon nanotube field-effect transistors," *Nature*, vol. 424, no. 9593, pp. 654–657, 2003.

[2] *International Technology Roadmap for Semiconductor 2005*. [Online]. Available: http://public.itrs.net

[3] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, "Electric field effect in atomically thin carbon films," *Science*, vol. 306, no. 5696, pp. 666–669, 2004.

[4] M. Y. Han, B. Özyilmaz, Y. Zhang, and P. Kim, "Energy Band Gap Engineering of Graphene Nanoribbons," *Phys. Rev. Lett.* , vol. 98, no. 20, p. 206 805, May 2007.

[5] M. C. Lemme, T. J. Echtermeyer, M. Baus, and H. Kurz, "A graphene field-effect device," *IEEE Electron Device Lett.*, vol. 28, no. 4, pp. 282–284, Apr. 2007.

[6] Z. Chen, Y.-M. Lin, M. J. Rooks, and P. Avouris, *Graphene Nano-Ribbon Electronics*. [Online]. Available: http://arxiv.org/abs/cond-mat/0701599

[7] Y. W. Son, M. L. Cohen, and S. G. Louie, "Energy gaps in graphene nanoribbons," *Phys. Rev. Lett.*, vol. 97, no. 21, p. 216 803, Nov. 2006.

[8] S. Reich, J. Maultzsch, C. Thomsen, and P. Ordejon, "Tight-binding description of graphene," *Phys. Rev. B, Condens. Matter*, vol. 66, no. 3, p. 035 412, Jul. 2002.

[9] Y. Ouyang, Y. Yoon, J. K. Fodor, and J. Guo, "Comparison of performance limits for carbon nanoribbon and carbon nanotube transistors," *Appl. Phys. Lett.*, vol. 89, no. 20, pp. 203 107–203 109, Nov. 2006.

[10] G. Liang, N. Neophytou, D. E. Nikonov, and M. S. Lundstrom, "Performance projections for ballistic graphene nanoribbon field-effect transistors," *IEEE Trans. Electron Devices*, vol. 54, no. 4, pp. 677–682, Apr. 2007.

[11] G. Fiori and G. Iannaccone, "Code for the 3D simulation of nanoscale semiconductor devices, including drift-diffusion and ballistic transport in 1D and 2D subbands, and 3D tunneling," *J. Comput. Electron.*, vol. 4, no. 1/2, pp. 63–66, Apr. 2005.

[12] G. Fiori, G. Iannaccone, and G. Klimeck, "A three-dimensional simulation study of the performance of carbon nanotube field-effect transistors with doped reservoirs and realistic geometry," *IEEE Trans. Electron Devices*, vol. 53, no. 8, pp. 1782–1788, Aug. 2006.

[13] J. Chen, T. Y. Chan, I. C. Chen, P. K. Ko, and C. Hu, "Subbreakdown drain leakage current in MOSFET," *IEEE Electron Device Lett.*, vol. EDL-8, no. 11, pp. 515–517, Nov. 1987.