Relevance of the physics of off-plane transport through 2D materials on the design of vertical transistors

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***Abstract*— We propose a theoretical study of vertical transport through graphene and two-dimensional materials, using simulations based on density functional theory and on pseudo atomistic Hamiltonians. We highlight the importance of interfaces and of band structure matching between adjacent layers, showing that graphene can offer a significant barrier to electron tunneling. We also show that the energy dependence of the transmission probability of other semiconducting two-dimensional materials is strongly affected by the details of the energy dispersion relations of the barrier and of the emitter and collector regions.**

***Keywords—tunneling; two-dimensional materials; graphene, vertical transistors*[1]**

I. INTRODUCTION

Since the first isolation and characterization of graphene in 2004 [1], its high mobility and single-atom thickness has made it an attractive material for electron devices for radio frequency applications. Graphene field-effect transistors (GFETs) have been fabricated and characterized with a cut-off frequency of few hundred gigahertz [2-4], but the lack of bandgap fundamentally limits the current modulation capability and the power gain (the so-called on/off ratio of the current is smaller than 10).

More recently, graphene devices based on off-plane (i.e., vertical) transport have been proposed [5-9] and demonstrated in experiments with very large current modulation between 10^4 and 10^5 [5], [9-11].

One of the most interesting of such devices is the graphene base transistor [7-8][11]: a thin graphene layer (acting as the base) is sandwiched between insulating or semiconducting layers (emitter and collector). As in the case of the hot electron transistors proposed in the eighties, the carrier injection in GBT is controlled by the emitter-base voltage which modulates the barrier height. Graphene thinness and high mobility should provide small base transit time and series resistance.

Other types of vertical devices have been proposed, that exploit graphene as the emitter and/or collector electrode [5],[9]. In those cases vertical transport is across dielectric or semiconducting layers, but not across graphene. They exploit graphene's finite (and relatively small) density of states, by virtue of which an electric field penetrates beyond a graphene sheet, with only partial attenuation. Indeed, in such types of vertical devices, the controlling electrode (gate) is separated from the controlled region (the barrier) by a graphene electrode, and therefore control is possible exactly because graphene cannot completely screen the electric field.

However, the partial screening of the electric field induced by the gate, due to the graphene electrode, undermines the efficiency of the electrostatic control mechanism. For this reason, [12] has shown such types of vertical devices have an intrinsically poor performance, due to the very mechanism of operation, and – even in ideal conditions - sub perform silicon devices by several orders of magnitude in terms of both delay times and power-delay product.

Let us stress the fact that GBTs exploit graphene properties in a different way as compared to planar devices (FETs). Planar devices take advantage of high mobility as a way to increase transistor beta, and therefore transconductance, gain, and cutoff frequency. On the other hand, GBTs use graphene thinness as a way to obtain short transit regions from emitter to collector, and therefore small transit time. They also use graphene mobility to reduce the base resistance, which has a direct impact on the voltage gain and on f_{max}.

Little is known about vertical transport through graphene and two-dimensional materials, both in terms of experiments and theory. The purpose of our work is to gain physical insights of the details of off-plane transport through graphene and two dimensional materials from the theoretical point of view, in order to support the design of transistors for digital or high frequency operations based on this transport mode.

II. TRANSPORT THROUGH GRAPHENE

First we investigate transport across the vertical semiconductor-graphene-semiconductor heterostructures by pseudo atomistic tight-binding simulations, considering several semiconductor materials (GaAs, GaN and Si) [13].

We have to consider that graphene and semiconductors are not lattice matched, and that alignment between different layers is not controlled in practice. For this reason, we use a pseudo-atomistic Hamiltonian for the semiconductor, with a pseudo-lattice that is matched to graphene, and with inter-atomic tight-binding hopping matrix elements (s_x, s_y, s_z) that allow us to fit the semiconductor energy dispersion relations around conduction band minima and valence band maxima (Fig. 1).

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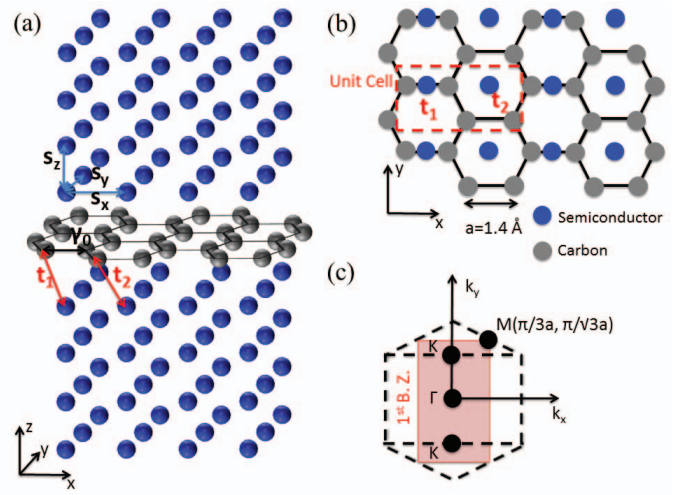

Fig. 1 (a) Vertical semiconductor-graphene-semiconductor heterostructure with pseudo semiconductor atoms (blue) and carbon atoms (grey). The blue arrows denote the inter-atomic tight-binding hopping matrix elements s_x, s_y, s_z in the semiconductor, and the red arrows denote the hopping parameters t_1, t_2 between the semiconductor and graphene. The carbon-carbon hopping parameter in graphene is γ_0 =-2.7 eV. (b) Top view of the structure with a unit cell consisting of four carbon atoms and two pseudo semiconductor atoms. (c) The first Brillouin Zone (B.Z., red) with high symmetry points Γ, K, and M.

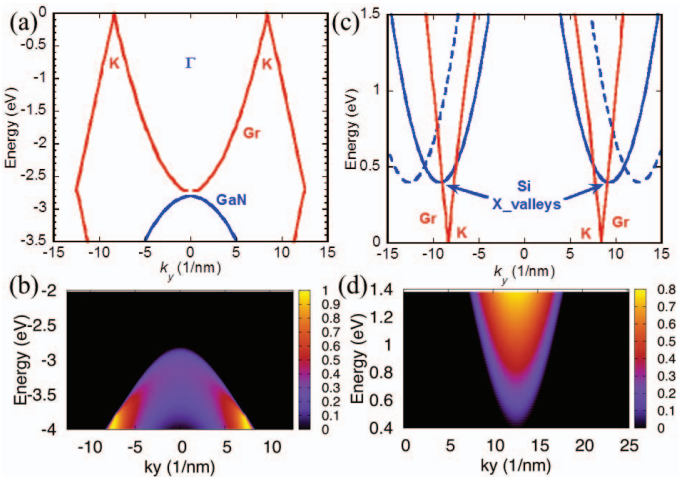

Fig. 2 a) Valence band dispersion along the k_y direction for graphene (tight-binding, red) and zinc-blende GaN (100) (2-band effective mass approximation, blue) for k_x = 0 and k_z = 0. (b) Transmission coefficient through the valence band of the vertical GaN-graphene-GaN heterostructure, with t_1 = -0.3 eV and t_2 = -0.2 eV, for k_x = 0. (c) Conduction band dispersion along the k_y direction for graphene (tight-binding, red) and Si (2-band effective mass approximation, blue solid). The blue dashed line is applied in the model for simplicity. (d) Transmission coefficient through the conduction band of the vertical Si-graphene-Si heterostructure, with t_1 = -0.3 eV and t_2 = -0.2 eV, for k_x = 0.

Graphene is described with the classic first-neighbor tight-binding Hamiltonian of graphene (carbon-carbon hopping parameter γ_0 =-2.7 eV). Coupling between the semiconductor and graphene is described by two hopping parameters t_1, t_2, which can be modulated to explore the impact of the degree of coupling between layers.

We find that the graphene layer cannot be simply treated as a transparent barrier. The vertical transmission coefficient can be greatly influenced by the coupling between graphene and the semiconductor layers, and also by the overlap between their energy dispersion relations in the k-space. For example, holes injected from Gallium Nitride (Fig. 2a) around the Γ point, find allowed states in the valence band of graphene, and therefore their tunneling probability can be relatively high. In the same way, electrons injected from silicon close to four of the six conduction band minima are injected close to the K point in graphene, where the graphene gap is zero, and can therefore be transmitted with high probability (Fig. 2b). Electrons in the other two silicon conduction band minima encounter a relatively high potential barrier.

On the other hand, semiconductors with medium bandgap and conduction band minima in the Γ point, such as for example GaAs, inject electrons at a point in the k-space where graphene represents a high, though thin, potential barrier. In those cases, the transmission probabilities can be rather small, depending on the values of t_1 and t_2.

Indeed, transmission probabilities are strongly dependent on the value of the hopping parameters t_1 and t_2 between different layers, which in turn depend on the fabrication process, and should therefore be strictly controlled to ensure the highest transparency of the barrier.

The relevance of this observations for device development is that **materials and interface matching has to be considered very carefully to optimize vertical transport**. From the modeling point of view, it is important not to assume that graphene is transparent to electrons and holes coming from off-plane directions, and to find indirect ways to extract the transmission probability or the degree of coupling between layers by fitting transport properties of specific test structures (e.g. semiconductor-graphene diodes).

There are other issues related to transport through graphene that we have not considered here: one is the very small forward current gain that is observed in experiments, which is typically of order 10^{-2}-10^{-3} [10-11]. Apparently, the large majority of injected carriers do not reach the collector but "recombine" in the base. The detailed causes of this phenomenon are not clear, and could either depend on an undesired emitter current component due to carriers injected at energy corresponding to the collector bandgap, for example through defect-assisted tunneling, or on carriers losing kinetic energy in their interaction with the graphene lattice. Specific characterization experiments are needed to gather more information and to completely understand this issue.

III. Transport Through Hexagonal Boron-Nitride

We have used first-principle density functional theory (DFT) to study the transport properties of single and double

barrier heterostructures realized by stacking between graphite leads layers of hexagonal BN or BC_2N, and graphene (Fig. 3). The heterostructures are lattice matched. The considered single barrier systems consist of layers of up to five h-BN or BC_2N atomic layers (with Bernal stacking) between graphite electrodes, as shown in Fig. 3. The scattering region considered in the calculation includes at least four atomic layers of graphite on each side of the barrier film, to ensure that the charge density does not change at the interface between the lead and the scattering region.

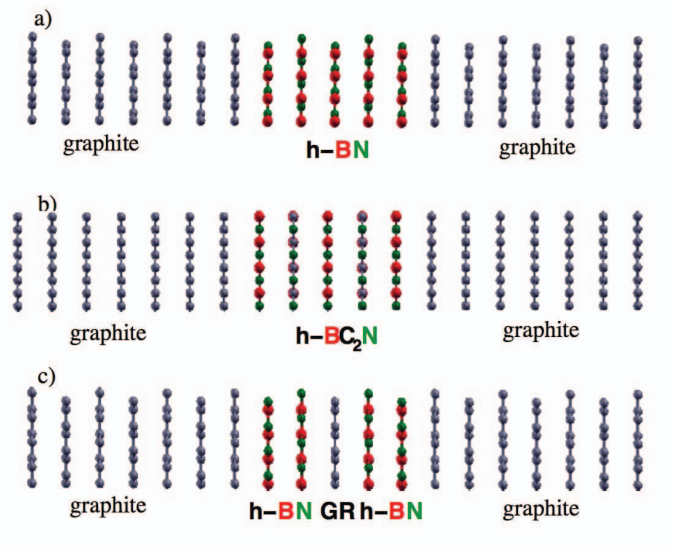

Figure 3: Side view of the supercell used to represent the scattering region corresponding to **a)** graphite—5(BN)—graphite; **b)** graphite—5(BC2 N)—graphite; **c)** graphite—2(BN)—graphene—2(BN)—graphite.

Ab-initio calculations have been performed by means of Quantum Espresso [14], using a plane wave basis set in the local density approximation (LDA). A 35 Ry wave function cutoff has been considered, the Brillouin zone has been sampled using a 30x30 Monkhorst-Pack grid. The geometry of the total system has been optimised with the van der Waals interaction-corrected density functional, as implemented in the Quantum Espresso code. Self-consistent calculations have been performed with the DFT-LDA method [15].

The transmission probabilities have been calculated with the PWCOND [16] module of Quantum Espresso. The transport properties are described in the framework of Landauer formalism. All details are reported in [15].

The transmission probability T of an h-BN barrier with different number of layers is plotted in Fig. 4 as a function of energy. It exhibits two peculiar behaviors:

- T is rather low also in a classically allowed energy region, due to a crystal momentum mismatch between states in graphite and in the dielectric layer.
- T is only weakly dependent on energy in the h-BN gap, because the imaginary part of the crystal momentum of h-BN is almost independent of energy.

As expected, the transmission probability decays exponentially with increasing n, as can be verified by plotting the average of T in the h-BN gap (energy between the Fermi energy E_{FERMI} and E_{FERMI} + 3.4 eV) as a function of the number of layers (inset of Fig. 4). The same considerations apply to a single barrier of hexagonale BC_2N (gap of 1.6 eV) of n atomic layers between graphite leads [15].

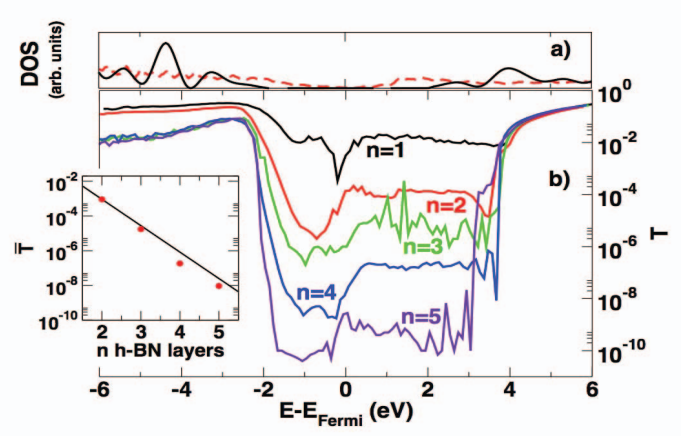

Figure 4: **a)** Density of states of bulk h-BN (solid black line) and graphite (dashed red line). **b)** Tunneling probability T of an h-BN barrier with n layers as a function of energy. Inset: average of T in the gap for an h-BN barrier of n atomic layers.

The impact of these consideration transistor design is that deep-energy tunneling is relevant in transport through two-dimensional materials, but simple WKB tunneling formulas would lead to strong underestimation of tunneling.

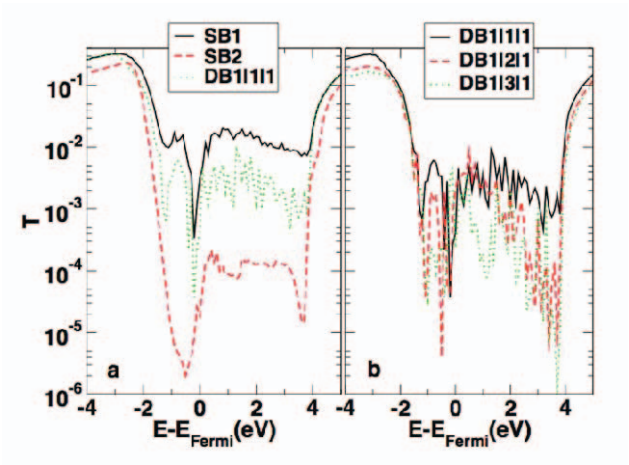

Figure 5: Transmission probability as a function of the energy (eV) for different systems; **a:** SB1 (solid black line), SB2 (dashed red line), DB1|1|1 (dotted green line). **b:** DB1|1|1 (solid black line), DB1|2|1 (dashed red line), DB1|3|1 (dotted green line).

Fig. 5 shows the transmission probability as a function of energy for some single and double barrier structures. All these systems are symmetrical, with two identical barriers separated by one, two, or three graphene layers. We denote the single barrier systems with the acronym SB followed by the number of h-BN layers, and the double barrier systems with DB and

three numbers, namely the number of h-BN layers on the left, the number of graphene layers in the central region, and the number of h-BN layers on the right.

There are two noteworthy aspects in transport through double barriers that are not typically seen in different materials systems, such as for example III-V semiconductor heterostructures:

1. It is apparent from Fig. 5a that the insertion of a single graphene sheet has a noticeable effect of transport: the transmission probability of a triple layer with a graphene layer inserted between two h-BN sheets (DB1-1-1) is much higher than that of a single layer with two h-BN sheets (SB2).
2. No resonant tunneling occurs in the double barrier structures.

Both aspects are due to the fact that the energy dispersion relation in graphene cannot be expressed as the sum of a longitudinal and a transversal component. For different transversal components of the crystal wavevector, clear resonant transmission peaks are present, but at different energies. They are therefore averaged out in the sum over all transversal wavevectors, so that no resonance is visible in the total transmission, and the only effect is an average higher transmission probability with respect to a single barrier with the same number of layers.

IV. Conclusion

Complete understanding of vertical transport through graphene and other two-dimensional materials require an atomistic approach, because interaction between layers and matching of energy dispersion relations have a strong effect on transport. We have performed both first principle and pseudo-atomistic simulations of transport through vertical structures, and we have achieved a set of insights that are especially relevant for the operation of vertical graphene-based transistors. We summarize them below:

- Graphene cannot *a priori* be considered as fully transparent to electrons and holes injected from off-plane directions. Both the quality of the interface between graphene and the emitter and collector layers, and bandstructure matching are very important in determining the device transport properties
- The details of the energy dispersion relations in semiconducting or insulating two-dimensional materials have a strong effect on the energy dependence of tunnelling. Simple approximations such as WKB can lead to significant errors, also from the qualitative point of view.
- The approximation of decomposing the Hamiltonian of the few atomic layer barrier in a longitudinal and a transversal component can lead not just to quantitative but also to qualitative errors (for example, it can lead to predict a non-existing resonant tunnelling component).

Several other issues are still open, mainly related to the availability of simple physical models, and to a full understanding dissipative mechanisms in vertical transport. For many of these aspects, systematic and dedicated experiments are very much needed.

References

[1] 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, pp. 666–669, 2004.

[2] Y. -M. Lin, C. Dimitrakopoulos, K. A. Jenkins, D. B. Farmer, H. -Y. Chiu, A. Grill, Ph. Avouris, "100-GHz transistors from wafer-scale epitaxial graphene," Science, vol. 327, pp. 662, Feb. 2010.

[3] L. Liao, Y. -C. Lin, M. Bao, R. Cheng, J. Bai, Y. Liu, Y. Qu, K. L. Wang, Y. Huang, and X. Duan, "High-speed graphene transistors with a self-aligned nanowire gate," *Nature*, vol. 467, no. 7313, pp. 305–308, Sep. 2010.

[4] Y. Wu, Y. -M. Lin, A. A. Bol, K. A. Jenkins, F. Xia, D. B. Farmer, Y. Zhu, and P. Avouris, "High-frequency, scaled graphene transistors on diamond-like carbon," *Nature*, vol. 472, no. 7341, pp. 74–78, Apr. 2011.

[5] L. Britnell, R. V. Gorbachev, R. Jalil, B. D. Belle, F. Schedin, A. Mishchenko, T. Georgiou, M. I. Katsnelson, L. Eaves, S. V. Morozov, N. M. R. Peres, J. Leist, A. K. Geim, K. S. Novoselov, L. A. Ponomarenko, "Field-effect tunneling transistor based on vertical graphene heterostructures," *Science*, vol. 335, no. 6071, pp. 947-950, Feb. 2012.

[6] G. Fiori, S. Bruzzone, and G. Iannaccone, "Very large current modulation in vertical heterostructure graphene/hBN transistors," *IEEE Trans. on Electron Devices*, vol. 60, no. 1, pp. 268-273, Jan. 2013.

[7] W. Mehr, J. Dabrowski, J. C. Scheytt, G. Lippert, Y, -H Xie, M. C. Lemme, M. Ostling, and G. Lupina, "Vertical graphene base transistor," *IEEE Electron Device Lett*., vol. 33, no. 5, pp. 691-693, May 2012.

[8] B. D. Kong, C. Zeng, D. K. Gaskill, K. L. Wang, K. W. Kim, "Two dimensional crystal tunneling devices for THz operation," *Appl. Phys. Lett.*, vol. 101, pp. 263112, Dec. 2012.

[9] H. Yang, J. Heo, S. Park, H. J. Song, D. H. Seo, K. –E. Byun, P. Kim, I. Yoo, H. –J. Chung, and K. Kim, "Graphene barristor, a triode device with a gate-controlled Schottky barrier," *Science*, vol. 336, no. 6085, pp. 1140-1143, May 2012.

[10] C. Zeng, E. B. Song, M. Wang, S. Lee, C. M. Torres, J. Tang, B. Weiller, and K. L. Wang, "Vertical graphene-base hot-electron transistor," *Nano Lett*., vol. 13, no. 6, pp.2370-2375, May 2013.

[11] S. Vaziri, G. Lupina, C. Henkel, A. D. Smith, M. Ostling, J. Dabrowski, G. Lippert, W. Mehr, and M. C. Lemme, "A graphene-based hot electron transistor," *Nano Lett*., vol. 13, no. 4, pp. 1435-1439, Mar. 2013.

[12] D. Logoteta, G. Fiori, G. Iannaccone, "Graphene-based lateral heterostructure transistors exhibit better intrinsic performance than graphene-based vertical transistors as post-CMOS devices" Vol. 4, Scientific Reports, pp. 6607-6614, 2014

[13] Q. Zhang, G. Fiori, G. Iannaccone, "On Transport in Vertical Graphene Heterostructures", IEEE Electron Device Letters vol. 35, n. 9, pp. 966-968, 2014.

[14] P. Giannozzi et al., "Quantum Espresso: a modular and open-source software project for quantum simulations of materials", J. Phys.: Condens. Matter vol. 21, art. n. 395502, 2009.

[15] S. Bruzzone, G. Iannaccone, G. Fiori, "Transport through hexagonal boron-nitride", arxiv:1212.4629

[16] A. Smogunov, A. DalCorso, and E. Tosatti, "Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials", Phys. Rev. B vol. 70, art. n. 045417, 2004.