Perspectives of graphene nanoelectronics: probing technological options with modeling

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Abstract

In this paper we show how numerical and analytical modeling of graphene-based devices is used to consider possible approaches to engineer a gap in graphene and to evaluate the perspectives of different technological options towards graphene nanoelectronics.

Introduction

Among the many unique structural and electronic properties of graphene, some are very promising for nanoelectronic applications [1], such as room temperature mobility much larger than that of bulk silicon. However, even assuming that many manufacturing challenges will be overcome with technology development, graphene also presents a serious problem and a possible showstopper for electronic applications: it has a zero bandgap.

Transistors and diodes need to be made of a semiconductor with a gap sufficiently large to suppress interband tunneling, that can undermine the possibility of switching the device off. For this reason, several options for inducing a gap in graphene have been pursued in recent years, with partial success, at least from the point of view of manufacturability of large scale integrated circuits.

Especially when a fabrication technology is in its infancy, as in the case of graphene, modeling can be a very powerful tool to evaluate the perspectives of different technology options. First, one has to be optimistic, and assume that fabrication techniques will improve to a point in which the ideal devices we dream of can be realized. Then, one can use modeling to answer some hard questions: what's their potential performance? How would they compare to CMOS devices? What would be their intrinsic limitations? Do we foresee any intrinsic manufacturability issue? Can we support (or guide) experimental developments?

In this paper, we will show how modeling has been used to address these issues, and in particular to evaluate different options to engineer a reliable gap in graphene FET channels. Numerical transport simulations have been performed with a 3D atomistic NEGF solver developed in Pisa, now freely available with a BSD open source license [2].

Bandgap engineering for graphene-based FETs

Different options can be considered for inducing a bandgap in graphene: *i)* lateral confinement, i.e., using graphene nanoribbons as material for FET channels, *ii)* the use of bilayer graphene, that has a gap tunable with a perpendicular electric field, *iii)* the use of epitaxial graphene on SiC, *iv)* graphene functionalization or doping. In the following of this section, we will discuss the potential of these options, evaluated through modeling.

Graphene nanoribbons
Nanoribbons offer a very interesting advantage over carbon nanotubes: as can be seen in Fig. 1, by virtue of edge relaxation, all nanoribbons have a semiconducting gap [3].
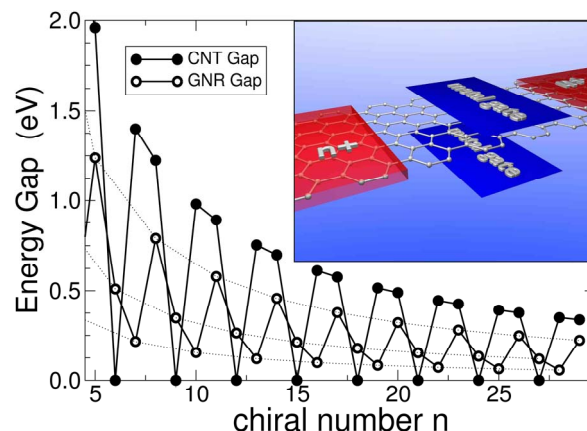

Fig. 1: Energy gap as a function of the chiral number in zigzag carbon nanotubes (2n,0) [black] and in zigzag carbon nanoribbons (2n, 0) [white].

However, the gap undergoes huge changes for a width variation corresponding to a single dimer. This means that reproducibility of the transfer characteristics requires single atom control: for example the double-gate FET shown in the inset of Fig. 1 (gate length 15 nm, oxide thickness 2 nm) exhibits the DC characteristics shown in Fig. 2 when the dimer number changes by only one [4]. Furthermore, a (12,0) nanoribbon has a width of 1.37 nm, still prohibitive from the fabrication point of view.

A non-ideality factor such as edge roughness can soften the dependence of the DC characteristics on the atomistic width of the nanoribbon, but suppresses mobility and therefore the on-current, and at the same time increases the off-current because the subthreshold slope is degraded due to the spatial modulation of the gap [5]. The same considerations can be made when dissipative transport in the channel is taken into account with a semi-analytical device model [6].
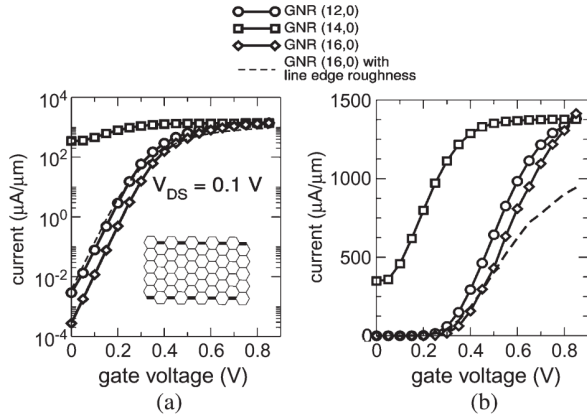
Fig. 2: Transfer characteristics of GNR-FETs in (a) logarithmic and (b) linear scale. Different nanoribbons are considered: (12,0), (14,0), and (16,0), V_{ds} = 0.1 V. Dashed line: Transfer characteristics for the (16,0) GNR-FET when roughness at the lateral edge of the GNR is considered. From [4].
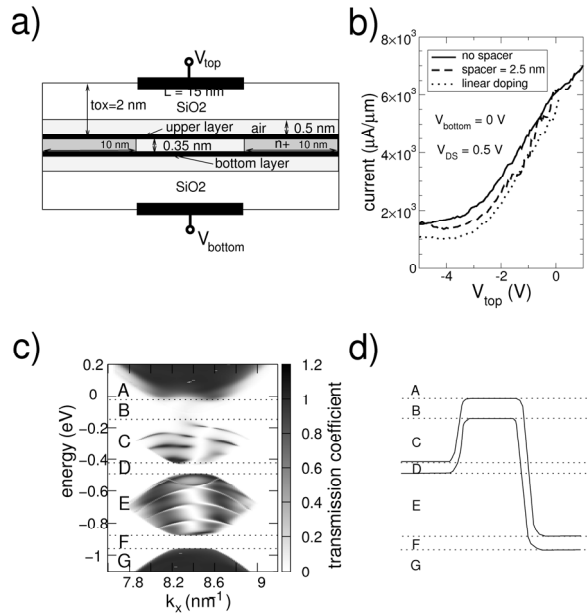

Fig. 3. a) structure of the double-gate bilayer graphene FET; b) transfer characteristics for V_{ds} = 0.5 V; c) Transmission coefficient of bilayer graphene channel as a function of energy and transversal k; d) band profile corresponding to c). From Ref. [13].
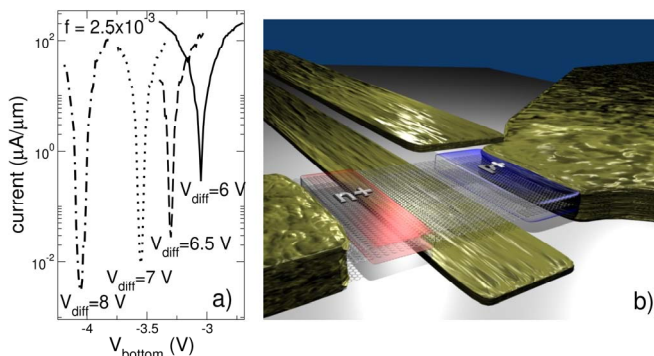

Fig. 4: Left: transfer characteristics of a double-gate bilayer graphene TFET for V_{ds} = 0.1 V, and for different differential voltages applied to the two gates [16]. The device is sketched on the right: channel length of 15 nm, gate overlap on source and drain extensions of 20 nm, oxide thickness 3 nm.

Bilayer graphene FETs and Tunnel FETs

In bilayer graphene the gap can be tuned through the application of a vertical electric field, as predicted theoretically [7,8] and observed experimentally [9,10]. This fact opens an interesting possibility: one could devise a device in which the bandgap becomes large only when needed, i.e., when the device should be in the off state.

In addition, bilayer graphene is a two-dimensional channel, requiring no prohibitive lithography. Bilayer graphene FETs have been investigated with top-of-the-barrier [11] or analytical models [12]. The first tight-binding atomistic simulations have been performed in [13], taking into account the details of gap tunability and interband tunneling, that is the main limitation to the use of small gap devices. However, while in principle one could obtain a gap of roughly 0.3 eV, in practice charge screening suppresses the maximum potential difference between the two monoatomic layers, and it is very difficult to obtain a gap larger than 0.15 eV (Fig. 3c). In this situation, interband tunneling dominates the off state, and current modulation is extremely poor when a reasonable supply voltage V_{dd}=0.5 V is considered (Fig. 3b) for a FET. Exploration of the design space of bilayer graphene FET with an ad-hoc semi-analytical model [14], has allowed us to assess that the maximum achievable I_{on}/I_{off} ratio is close to 10 for a supply voltage of 0.5 V, largely insufficient for integrated circuit applications (the ITRS 2008 requires a I_{on}/I_{off} > 10^4 for V_{dd} = 0.5 V) [15].

The interband tunneling current and the subthreshold swing strongly depend on the applied $V_{ds}=V_{dd}$. Let us consider an nFET: the larger V_{ds}, the stronger the interband tunneling, which directly contributes to the off-current, and the higher the injection of holes in the channel, which in turn increases the channel quantum capacitance and degrades the subthreshold swing [4]. In the case of a FET, V_{dd} can be hardly reduced because the ideal subthreshold swing at room temperature is 60 mV/decade, so that an I_{on}/I_{off} ratio of 10^4 requires a supply voltage of at least 0.24 V.

The situation can be more favorable with a Tunnel FET, where the subthreshold swing can be smaller, enabling the use of a much smaller V_{dd}. Tunnel FETs realized with carbon nanotubes have been demonstrated [16], and simulations have been presented of TFETs with graphene nanoribbon channels [17-18]. However, the poor control of the energy gap of 1D carbon channels is even more severe in the case TFETs, whose behavior critically depends on the tiny region close to the source where interband tunneling takes place.

The gap of a 2D sheet of bilayer graphene only depends on the vertical electric field, and this can be a significant advantage. We have simulated the operation of ideal double-gate or single-gate ballistic devices and a V_{dd} of only 0.1 V [19].

One can see in Fig. 4 that in the case of a differential voltage of 8 V applied between the two gates in order to induce an energy gap, one can obtain a I_{on}/I_{off} ratio close to 10^4 with a supply voltage of only 0.1 V, thanks to a subthreshold swing smaller than 20 mV/decade.
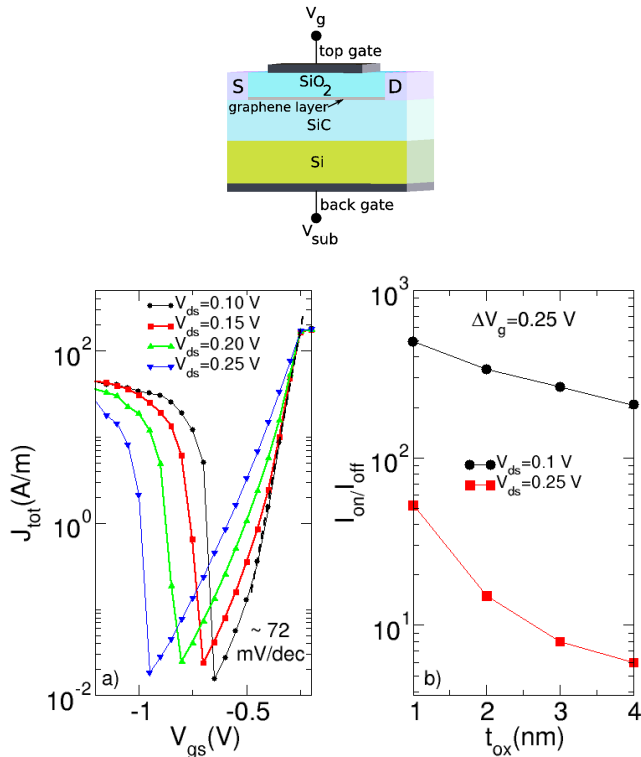
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Fig. 5: Top: illustration of the epitaxial graphene on SiC FET. Left: transfer characteristics of a FET based on epitaxial graphene on SiC for different values of V_{ds}, showing the degradation of the subthreshold slope with increasing V_{ds}. Right: I_{on}/I_{off} ratio as a function of the oxide thickness.

I_{on}/I_{off} ratio of up to 10^4 with a supply voltage of 0.2 V.

Functionalized Graphene

Chemical functionalization of graphene sheets or graphene nanoribbons is a very promising option for tuning the bandstructure and the electronic properties. Recent experiments have shown that conductance variations of up to six orders of magnitude can be obtained by reversible chemical modifications (probably hydrogenation) suggesting the possibility of realizing memory elements [22]. More recently, the experimental demonstration of graphane [23], a two-dimensional hydrocarbon with a gap of 4-5 eV obtained by hydrogenation of graphene via plasma treatment, has further proven that chemical functionalization is a viable route toward bandgap engineering of graphene-based materials. However, appropriate methods to attain good ohmic contacts and to retain high mobility (exceeding 100 cm^2/Vs) are still needed.

From a modeling point of view, investigating the possibility offered by chemical functionalization of graphene requires researchers to combine the traditional methods of quantum chemistry for the ab-initio simulation of material properties with the tools typically used for the study of charge transport in nanoscale conductors.

A recent first-principle computational study [24] shows that substitutional boron doping can induce a mobility gap as large as 1 eV even in 10 nm-wide nanoribbons. A mobility gap is different from an energy gap, and it remains to be understood whether it is capable to suppress interband tunneling, which is the reason an energy gap is needed in the first place.

A different study [25], is based on using density functional calculations of graphene clusters with boron dopants, such as those shown in Fig. 6a and 6b, to extract tight-binding parameters of boron-doped graphene. These parameters are then used to simulate nanoribbon FETs with an NEGF-based transport code [2]. One lesson is that the position of boron atoms strongly affects the obtained bandgap: for example, the structure in Fig. 6c has a bandgap of 0.6 eV, whereas the structure in Fig. 6d has a bandgap of only few tens of meV. In addition, boron doping strongly suppresses nanoribbon mobility, and therefore a more convenient approach could consist in doping the nanoribbon edges, where impurities have a smaller effect on mobility. Boron doping at the edges is in particular effective in opening a gap in quasi-metallic nanoribbons, and therefore could mitigate the sensitivity of the bandgap to width fluctuations.

Edge functionalization has been investigated also in Ref. [26], where graphene nanoribbon FETs with edges terminated with different species (H, O, OH, F) are simulated and compared in terms of performance. Band structures are computed with DFT, and a top-of-the-barrier model is used to compute the DC device characteristics. In this work, the effect of edge termination is not dramatic, even for very narrow wires (n=12), and H termination seems to be more

Bilayer graphene is really fit to the realization of TFETs: on the one hand, the small gap and small effective mass can allow to achieve a large on-current, compared with other material systems. On the other hand, the electronic structure is such that even 2D bilayer graphene has a small quantum capacitance, and therefore all the advantages of 1D TFETs in terms of subthreshold swing [19], but relative ease of patterning.

Epitaxial graphene on SiC

Recent experiments [20] have shown that a graphene layer grown by epitaxy on a SiC substrate can exhibit a gap of about 0.26 V, measured by angle-resolved photo-emission spectroscopy. Further experimental confirmation and reproduction of results are still needed, but the point is very interesting, because epitaxial graphene on SiC is promising for wafer scale fabrication. We have evaluated the possibility of using the material as FET channel, exploring the design space with a semi-analytical model [21]. An I_{on}/I_{off} ratio of up to 60 can be obtained for $V_{dd} = 0.25$ V, but the supply voltage (in V) cannot be larger than the channel bandgap (in eV), otherwise strong interband tunnelling cuts in. Large current modulation is possible for smaller V_{ds}, but again, if one consider digital applications, the applied V_{ds} must equal the V_{gs} swing.

As expected, preliminary results show that epitaxial graphene on SiC is promising for Tunnel FETs, exhibiting an

promising in terms of the on-current, and a balanced n-FET and p-FET performance.

Final Remarks

Numerical and analytical modelling is a powerful tool to explore several different options to induce a gap in graphene and to realize transistor structures, with the aim of assessing the actual potential of this material in electronics. This is a very significant role that modeling can play in the worldwide quest for towards carbon- and molecule-based electronics.

We have some concluding remarks: first, in order to exploit graphene in nanoelectronics on an industrial level, one has to find a new and reliable way to induce a significant gap in graphene. Graphene nanoribbons are not promising from a manufacturability point of view, because they require really prohibitive lithography and single-atom control. Bilayer graphene and epitaxial graphene on SiC have a gap of 0.1-0.3 eV, and therefore can be promising only for TFETs: experiments in this direction are under way but no transport result is available at the moment. In addition, the gap in epitaxial graphene on SiC needs to be confirmed, also with transport experiments, by more than one group. Finally, chemical modifications of graphene are an option for inducing a significant gap, but there is a trade-off with mobility degradation to be pondered very carefully.
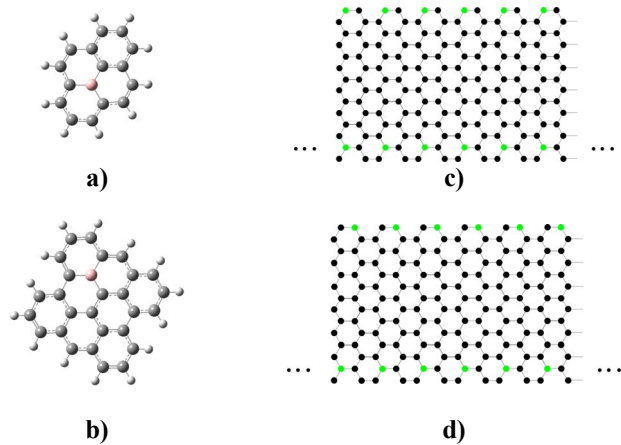
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Fig. 6: a) and b): graphene clusters with substitutional boron considered in the DFT simulations; c) and d) different boron edge decorations lead to different bandgaps: 0.6 eV in the case of c), few tens of meV in the case of d).

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