

Graphene Devices, Interconnect and Circuits – Challenges and Opportunities

Mircea R. Stan, Dincer Unluer, Avik Ghosh, Frank Tseng
Univ. of Virginia, ECE Dept., Charlottesville, VA 22904
{mircea,du7x,ag7rq,ft8e}@virginia.edu

Abstract—Graphene has recently emerged as a serious contender for the post Silicon era. Graphene NanoRibbon (GNR) devices have similar performance characteristics as Carbon Nano Tube (CNT) ones. However, lithographic patterning methods applied to graphene avoids the degree of chirality control and alignment issues typical of CNTs. GNR devices and GNR interconnect can be seamlessly obtained by patterning single graphene sheets thus leading to monolithically device-interconnect structures. Electrically doped GNR devices in series and in parallel can be used for creating complex GNR FET digital circuits. There are also several important challenges facing the graphene “brave new world,” but many of the difficulties hopefully will have tractable solutions. This paper examines the topic of GNR FET circuit design from a bottom-up theoretical perspective, starting with GNR device and interconnect modeling and simulation, while trying to reconcile theory with some recent experimental results.

Keywords: graphene nanoribbons, GNR, carbon nanotubes, CNT

I. INTRODUCTION

Two-dimensional graphene sheets have interesting electrical characteristics, related to those of Carbon Nano Tubes (CNTs) [1]. This paper investigates graphene sheets patterned into ribbons of given width and angle with respect to the two-dimensional hexagonal (honeycomb) lattice. Graphene Nano Ribbons (GNRs) [2] have either metallic or semiconductor behavior depending on their dimensions and orientation to the hexagonal graphene lattice. The paper discusses how to model GNRs and also investigates gating GNRs either with metallic plates, or with other graphene ribbons orthogonal to the device, in order to obtain devices with gain. Finally the paper tries to reconcile the theory with some recent experimental results that seem initially at odds with some early theoretical models. The approach used for the device modeling aspects of the paper combines the channel and contact band-structures with three-dimensional electrostatics and a treatment of quantum transport using the non-equilibrium Green’s function (NEGF) technique [3]. This is a significant departure from traditional transport simulation approaches based on continuum effective mass theory and classical drift-diffusion equations that are not valid at nanometer length-scales.

II. GRAPHENE ADVANTAGES

GNRs have electrical characteristics that are quite similar to CNTs (thus good performance). In principle, a nanoribbons planar features can be patterned using more standard semiconductor industry fabrication methods, which (a) *bypasses the alignment problem* that CNTs face, and (b) offers *control over the ribbon width and orientation* (and thus its metallicity). This is in contrast with CNTs, whose chiralities are predetermined statistically during the manufacture process and are near impossible to control.

A. Graphene Nano Ribbons – GNRs

The nomenclature for both GNRs and CNTs uses the terms “armchair” and “zigzag”, but, confusingly, in an opposite way. For CNTs the terms armchair and zigzag indicate the pattern of the tube *circumference*, while for GNRs the same terms indicate the pattern of the ribbon *edge*. Thus an *armchair* GNR can be visualized as an “unrolled” *zigzag* CNT, and *vice-versa*. See Fig. 1 for a graphic representation.

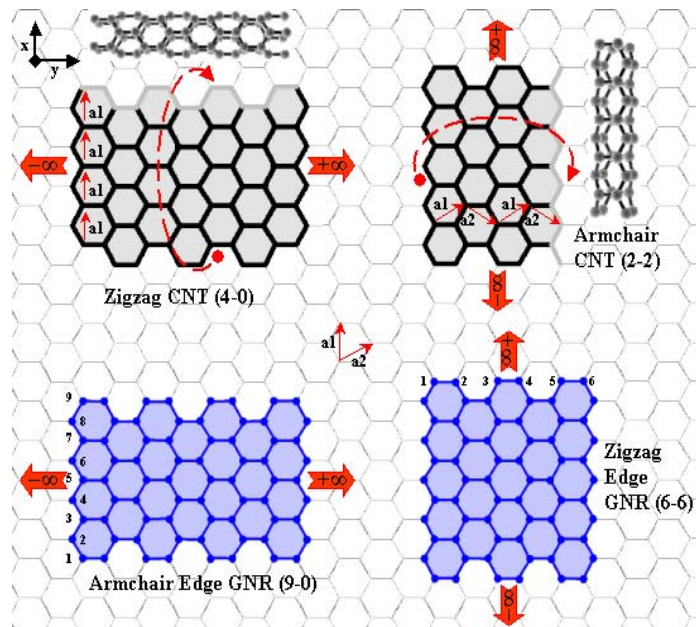


Fig. 1 Armchair edge GNRs are related to zigzag CNTs, left, and zigzag edge GNRs are related to armchair CNTs, right

B. Electrical characteristics

The carbon atoms in graphene are sp^2 hybridized and have strong links with their 3 nearest neighbors. The $2p_z$ atomic orbitals (AOs) of adjacent atoms in the graphene sheet overlap and form bonding (π -band) and anti-bonding (π^* -band) 2D bands. In the case of the CNTs, the *chiral* vector determines the way the energy levels are quantized, and the interaction between this quantization and the energy bands of the graphene determines the electrical characteristics of the CNT. Since many of the characteristics of CNTs stem from the underlying graphene lattice, it is expected that the electrical characteristics of a CNT will be maintained even when the CNT is unrolled into the equivalent GNR (which can be thought of as the planarized outer shell of the CNT, except that softer *fixed edge boundary conditions* on the ribbon replace more stringent *periodic boundary conditions* around the tube circumference.) This leads to lower band-gaps for GNRs while still preserving their overall chiral properties [8]. A first order analysis of graphene ribbons can follow almost the same methodology as that of CNTs. A 2D graphene hexagonal lattice [4] can be patterned into narrow ribbons that will create a (quasi)1D system with quantized states in the transversal direction. Tight-binding theory [10] is used to obtain E,k diagrams for GNRs, such as the (11,0) (no bandgap, i.e. semi metallic), and (7,0) (non-zero bandgap, i.e. semiconducting) armchair GNRs (AGNRs) in Fig. 2.

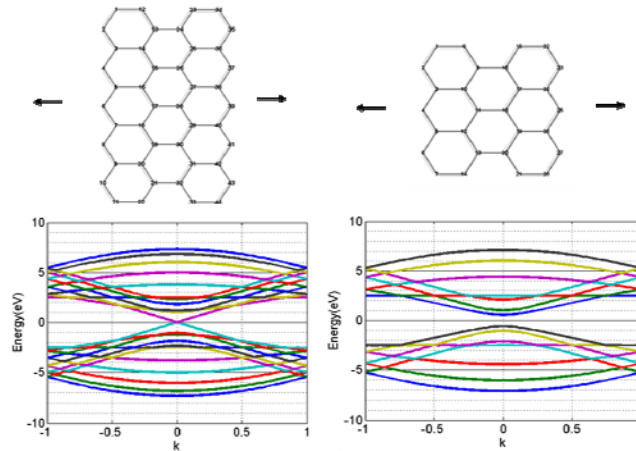


Fig. 2 E,k diagram for (11,0), left, and (7,0), right, AGNRs

The Extended Huckel theory (EHT) [5] can provide more detail in the band structure since it captures more of the chemistry. For example, Fig. 3 shows the E,k diagram for a (7,0) AGNR using EHT. The left side shows an unpassivated GNR, and the right side

shows an H-passivated one [9] clearly demonstrating the beneficial effect of H-passivation in eliminating deleterious edge states in the bandgap.

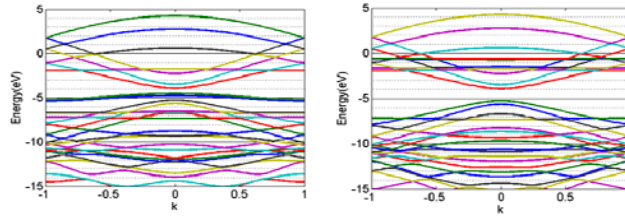


Fig. 3 (7,0) using EHT, unpassivated, left, passivated, right

C. “Monolithic” device-interconnect structures

The great potential and attraction of GNRs compared to CNTs is the possibility of obtaining “monolithic” device-interconnect structures by proper combinations of semiconducting and metallic regions that can seamlessly form entire circuits out of one patterned graphene sheet. Fig. 4 shows a combined structure example, in which a semiconducting (7,0) channel is “sandwiched” between semi metallic (11,0) source and drain, thus forming a transistor once a top and/or bottom gate is added. Clearly, the (11,0) metallic AGNRs can be extended to act as the interconnect. A very useful aspect of such combined structures is that, unlike CNTs, they don’t have any Stone-Wales defects [11] where the different regions join each other as can be also seen in Fig. 4.

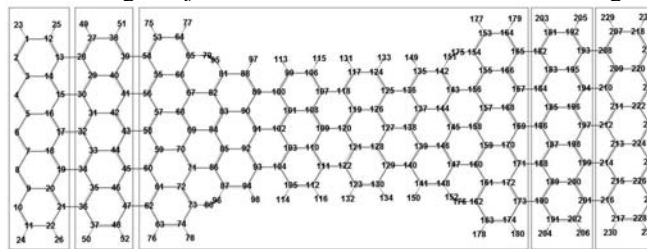
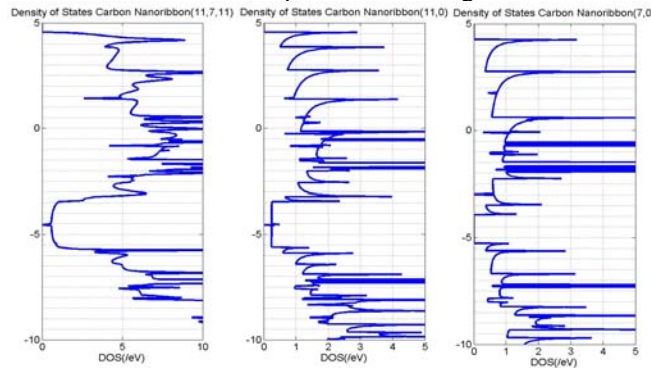


Fig. 4 “Monolithic” (11,7,11) AGNR device-interconnect

In order to determine if such monolithic structures have the right characteristics we used EHT and determined the density of states (DOS) and the transmission for AGNRs and for combinations of AGNRs. Fig. 5 shows that the DOS and transmission of the combined “monolithic” structures have their characteristics indeed dominated by the semiconducting regions, which is exactly what is needed in order to be able to obtain a transistor effect with a top and/or bottom gate.



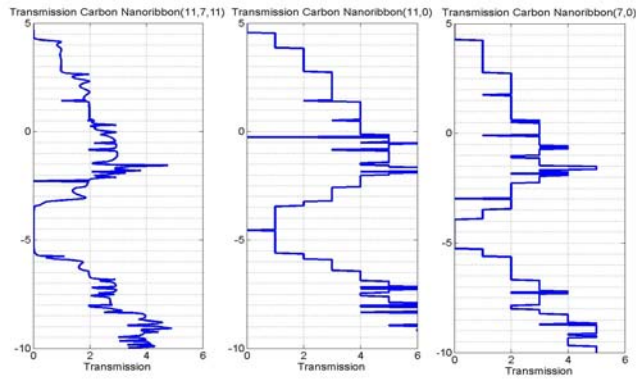


Fig. 5 Density of states, top, and transmission, bottom, for (7,0), right, (11,0), middle, and (11,7,11) combined, left

D. 2-D electrostatics

One big advantage of monolithic graphene devices is the 2D nature of the channel, source and drain regions. As opposed to the linear potential drops characteristic for 3D structures, 2D structures result in much steeper logarithmic drops. Ultimately this reduces short channel effects since the effect of the drain voltage over the channel drops more abruptly. Fig. 6 shows the Laplace potential in a monolithic AGNR device under three different bias conditions all illustrating better gate control over the channel compared to drain, and the steep drop in voltage typical of 2D electrostatics.

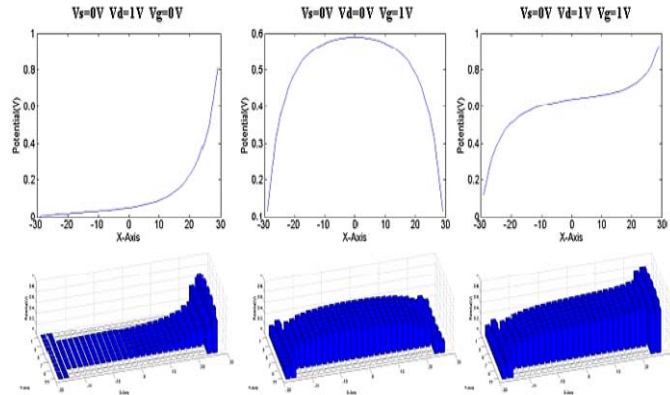
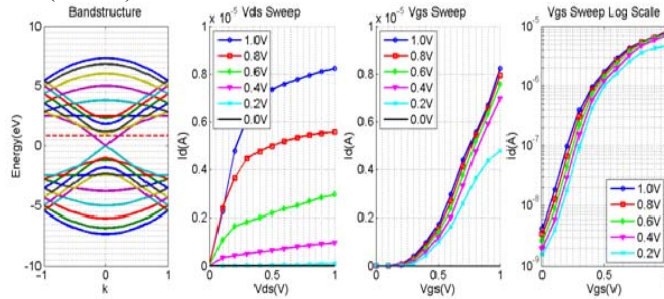


Fig. 6 Potential in AGNR device, *off* with 1V V_d s, left, *on* with 0V V_d s, middle, *on* with 1V V_d s, right

E. I-V characteristics

Due to symmetric valence and conduction bands GNR devices are intrinsically *ambipolar*. Shifting the Fermi level in the channel toward the conduction band (for NMOS) or the valence band (for PMOS) can be done using chemical and electrostatic doping methods, and/or gates with properly chosen gate workfunction values. Our formalism couples the electronic structure of graphene with Non-equilibrium green's function (NEGF) to obtain I-V characteristics for NMOS and PMOS AGNRs as seen in Fig.7



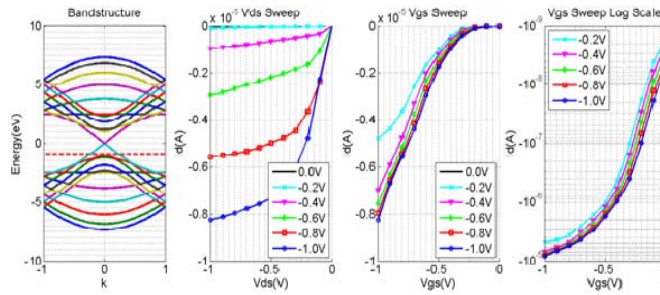


Fig. 7 I-Vds and I-Vgs for GNR NMOS, top, PMOS, bottom

III. GRAPHENE DIFFICULTIES

A. Fabrication and patterning

The possibilities of planar patterning GNRs are two-faced as this is a defining advantage, but also a drawback as long as the looming obstacles with nanoscale *top-down* lithography are not addressed. Currently, the requirement for atomic precision seems like another almost insurmountable difficulty. There is also a need for large-scale defect-free graphene wafers that has not been yet demonstrated, although there are promising steps in that direction [4].

B. Experiments vs. theory

A recent experimental paper [6] has raised questions about much of the early theoretical work related to GNRs. While the GNR theory predicts that AGNRs will have a semiconducting or semi-metallic behavior depending on the number of dimers across the width of the ribbon, i.e. $(3p,0)$ and $(3p+1,0)$ AGNRs are semiconducting, while $(3p+2,0)$ AGNRs are semi-metallic, the experiments in [6] showed that *all* narrow GNRs have bandgaps, while *all* wide GNRs are semi metallic!

IV. RECONCILING THEORY AND EXPERIMENTS

When theory and experiments do not agree it can mean that either the theory, or the experiments, or both, are “wrong”, or that the theory and the experiments really look at different structures. We try to reconcile theory with these recent experimental results by considering the following possible scenarios

A. EHT and DFT actually predict bandgaps for all GNRs

The first step is to consider more comprehensive theories than the simple tight indeed, both EHT and density functional theory predict non-zero bandgaps even for $(3p+2,0)$ AGNRs for which tight binding predicts a zero bandgap. Fig. 8 shows clearly the nonzero bandgap using EHT on AGNRs of increasing width. At close inspection the same small non-zero bandgap for a $(11,0)$ AGNR is also apparent in Fig. 5.

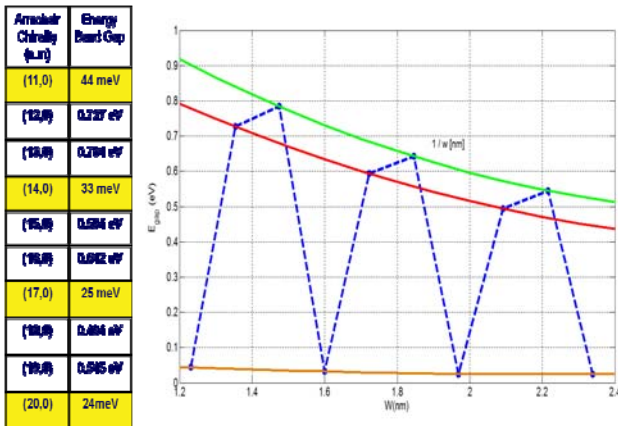


Fig. 8 Bandgap predicted by EHT for $(3p,0)$ AGNR, middle, $(3p+1,0)$ AGNR, top, $(3p+2,0)$ AGNR, bottom

Although this is a step in the right direction, it really does not fully reconcile with [6] since the bandgap for $(3p+2,0)$ AGNRs, while non-zero, is still much smaller than for the other two cases, so there must still be another explanation.

B. Effect of edge roughness

We postulate that the reason for the results in [6] is that, although “ultrasmooth,” the AGNRs measured in the experiments were not really *atomically smooth*. As we show in what follows, an edge roughness of even +/- one atom can significantly change the “transmission bandgap” of the GNR. In order to try to justify our hypothesis we have modeled several GNR structures with imperfect edges (missing atoms) as the ones in Fig. 9.

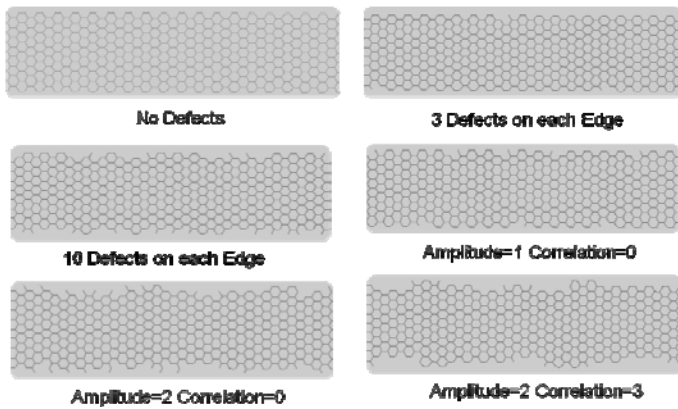


Fig. 9 AGNRs with increasing edge roughness

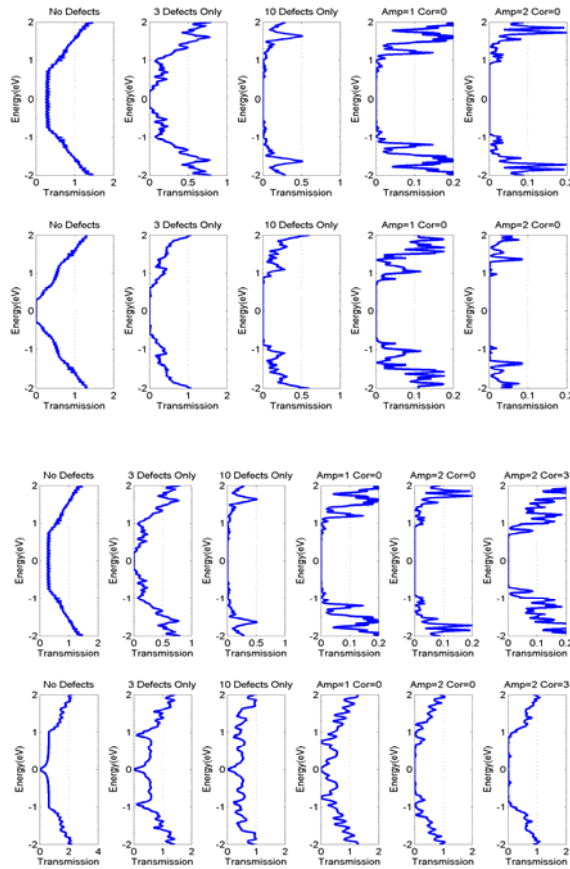


Fig. 10 Transmission for $(3p,0)$ vs. $(3p+2,0)$ narrow AGNRs with rough edges, top, and $(3p,0)$ AGNR vs. ZGNR, bottom

Fig. 10 shows the resulting transmission for the various GNR structures, with the ones without defects on the left side, and with gradually increasing edge roughness further to the right. The plots compare two types of narrow AGNRs, one of which starts as semi metallic when the edges are smooth, as well as an AGNR with a zigzag GNR (ZGNR), for which tight binding predicts as being always semi metallic. Fig. 10 clearly supports our hypothesis. As the edge roughness increases, all narrow GNRs, including those that start as semi metallic, even ZGNR, develop large “transmission bandgaps”, and become virtually indistinguishable as in [6]. How about wide GNRs? Fig. 11 shows that the effect of edge roughness on wide GNRs is negligible, and that the small bandgap collapses to zero for wide GNRs with or without edge roughness, making all of them semi metallic as in [6].

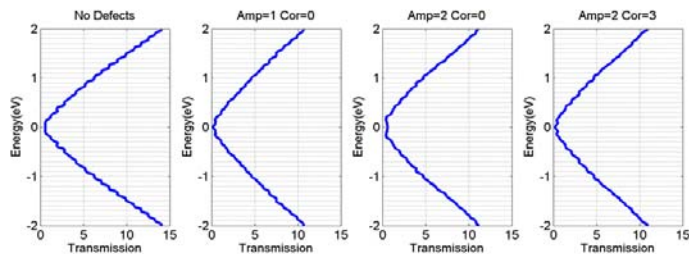


Fig. 11 Transmission (3p+1,0) wide AGNRs with rough edges

SUMMARY

Graphene is a promising material for future nanoelectronics. It has great electrical characteristics, is amenable to planar processing for getting monolithic device-interconnect circuits.

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