Toward models for CNT devices

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Abstract—**In the last decades it has been realized that scaling reaches the physical limits of the nowadays used materials. For this reason the semiconductor industry is looking for different materials and architectures to integrate with the current silicon-based technology or maybe, in a further future, even to substitute it. Amongst the plenty of solutions investigated, CarboNanoTubes(CNTs) are one of the more promising materials. They show a wide range of interesting features which can be exploited in principle to build both low-resistance high-strength interconnections and highly scalable low-power Field Effect Transistors and Single Electron Tunneling Transistors.**

In this paper we present an overview of the main experiments and applications that involve CNTs, explaining why their properties appear to be interesting for future electronic devices and how researchers are trying to exploit these properties to overcome technology related limitations for circuit manufacturing that are near to come.
Furthermore, we will discuss the possibility and some basic ideas to develop circuit models for the novel devices in order to make some steps from the actual research on physical level towards a circuit and system level approach. For this purpose, we will start to investigate the features that seem common to most of the experimental results presented till now. These features will be the basis for future models.

Keywords—**Nanoelectronics; energy band diagrams; CarboNanoTubes; interconnections; Field–Effect–Transistor.**

I. INTRODUCTION

In the last decades it has been realized that the scaling reaches the limits of the nowadays used materials [1]. In particular, the silicon based technology is now producing devices in which molecular and quantum effects are starting to influence and change the expected behavior, making the realization of good performance devices more and more difficult, if not impossible. For this reason the industry of semiconductors is looking for different materials and approaches to substitute or integrate with the current silicon-based technology.

Amongst the plenty of solutions proposed, CarboNanoTubes (CNTs) are one of the materials that are more interesting for integrating with or maybe, in a further future, substitute silicon-technology. They show a wide range of interesting features which can be exploited in principle to build both low-resistance high-strength interconnections and highly scalable low-power Field Effect Transistors and Single Electron Tunneling Transistors.

CNTs were discovered by Iijima [2] in 1991 while performing some experiments on molecular structures composed of carbonium. A CNT consists of a graphene sheet rolled up to form a cylindric molecule. It can be Single-Walled (SWNT) or Multi-Walled (MWNT), depending on how many walls the tube is made of. In Fig. 1 the structure of a graphene sheet together with a SWNT and a MWNT is shown.

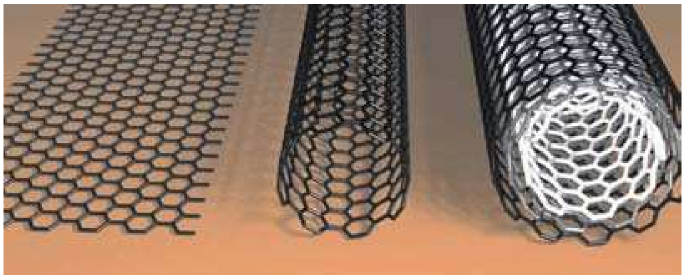

Fig. 1. *Illustration of a graphene sheet, a Single-Walled CNT and a Multi-Walled CNT.*

II. ELECTRIC PROPERTIES AND ENERGY BANDS DIAGRAMS

The electric properties of CNTs were investigated first by Hamada et al. using tight-binding band-structure calculations [3]. Their studies showed that CNTs properties are strongly dependent on their chirality and diameter. The chirality is related to the degree of the twist of the lattice of the tube and can be described by the chiral vector.

The chiral vector is a circular vector that is perpendicular to the axis of the tube. It is a linear combination of the base vectors $\vec{a_1}$ and $\vec{a_2}$. In mathematical terms the chiral vector is defined as:

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$$\vec{C} = n\vec{a}_1 + m\vec{a}_2 \tag{1}$$

where n and m are integers. In Fig. 2 a graphical representation of the chiral vector is shown. The vector $\vec{OA}$ has coordinates $(4, 2)$. Now, if we superpose the point A with the origin O, we obtain a $(4, 2)$ SWNT that will be made of the portion of lattice that is between the two lines OB and AB'. Sometimes the chiral vector is also defined using a linear coordinate and a angular coordinate referred to one of the base vectors. For instance in Fig. 2 the angle θ is referred to the base vector $\vec{a_1}$.

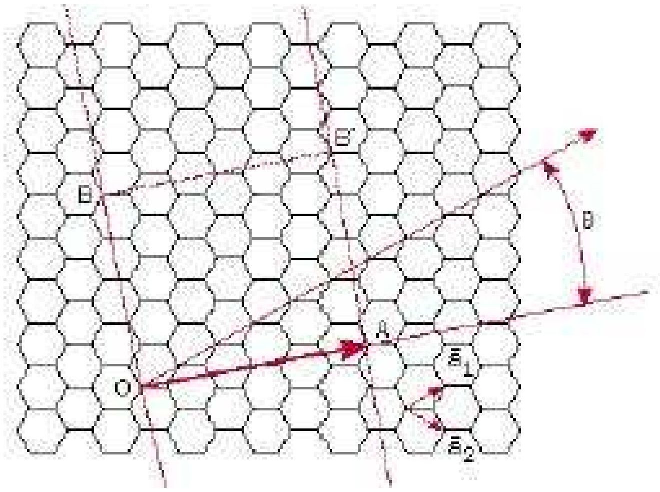

Fig. 2. *Definition of the chiral vector for a SWNT.*

In this way the couple of integers (n, m) defines the chirality and the diameter and therefore the position of the valence and conductance bands and consequently the value of the energy gap. Thus, depending to the couple (n, m), the SWNTs can have metallic or semiconducting behavior. In Fig. 3 an example of energy bands is shown for metallic and semiconducting SWNTs. An important condition to distinguish between the two categories is:

$$\frac{(2n + m)}{3} = \text{integer} \tag{2}$$

In particular, if equation (2) is not verified the SWNT will be certainly semiconductor-type. So the (2) is a necessary, but not sufficient, condition for the SWNT to be metallic. It has been demonstrated that SWNTs with the chiral vector of coordinates (n, n) are certainly metallic. In Fig. 4 some noticeable kinds of chiralities are shown with their respective names.

MWNTs are overall metallic. This is due to the fact that the coupling of the coaxial SWNTs contained in a MWNT doesn't appreciably change the band structure of the single tubes. This means that the tubes maintain their basic properties even if they are part of a MWNT. Thus, taking also into account the fact that in average one out of three SWNTs is metallic and that MWNTs have usually more than ten shells, we obtain in many cases metallic MWNTs because just one metallic SWNT is sufficient to short-circuit all the others semiconducting tubes [4].

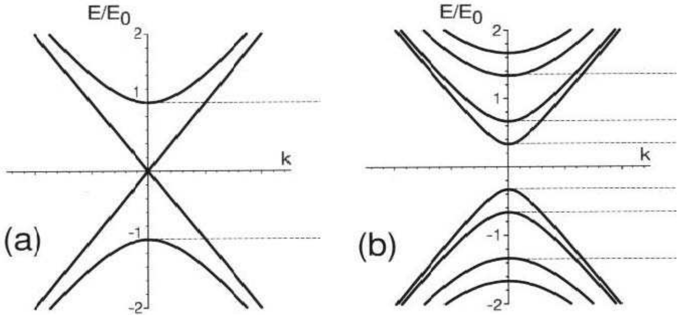

Fig. 3. *Energy bands in (a) metallic and (b) semiconducting SWNTs.*

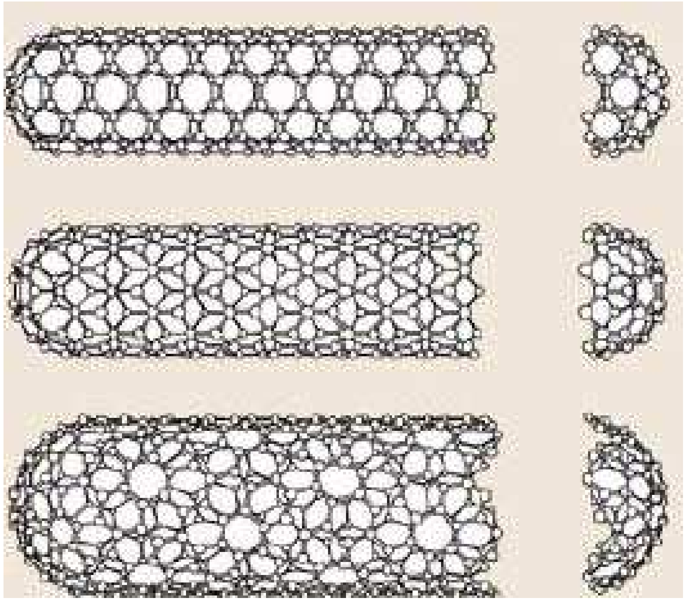

Fig. 4. *Different chiralities for different chiral vectors; from the top: armchair(5,5); zig-zag(9,0); chiral(10,5).*

Amongst the properties of metallic CNTs, much attention deserves also the property of conductance quantization. Indeed it has been shown that the perfect structure of the CNTs allows them to transport electrical charge without scattering over distances of up to several micrometers [5] in low-bias voltage. This property is called *ballistic transport*. Thank to this property, metallic CNTs show very low resistance, high current driving capabilities and almost no heat dissipation, features that can be exploited to build high-performance interconnections and devices for integrated circuits.

III. CARBONANOTUBES AS INTERCONNECTIONS

As we mentioned above, the ability of carbonanotubes to carry high current densities with a fixed resistance over lengths up to several micrometers makes them interesting for implementations of on-chip interconnections. Indeed it has been shown that they can carry till $10^{10}\ \frac{A}{cm^2}$, that is at least 100 times higher than the breakdown current for any metallic wire [6].

In the first experiments related to the conductive properties of CNTs, the conductance appeared to be quantized with a quantization unit equal to $G_0 = 2\ \frac{e^2}{h} = (12.9 \text{ kilohms})^{-1}$, where e is the electron charge and h is the Planck constant [5]. In following experiments a number of groups found out that at low temperatures and at low biases the conductance is approaching the value of 2 G_0. This effect has been attributed to the spin degeneracy that influences the conductance by a factor 2 [4]. In fig. 5 is shown the dependence of the differential conductance of a metallic CNT on the bias voltage at different temperatures. As said above, if the temperature decreases, the value gets closer to the predicted value of 2 G_0.

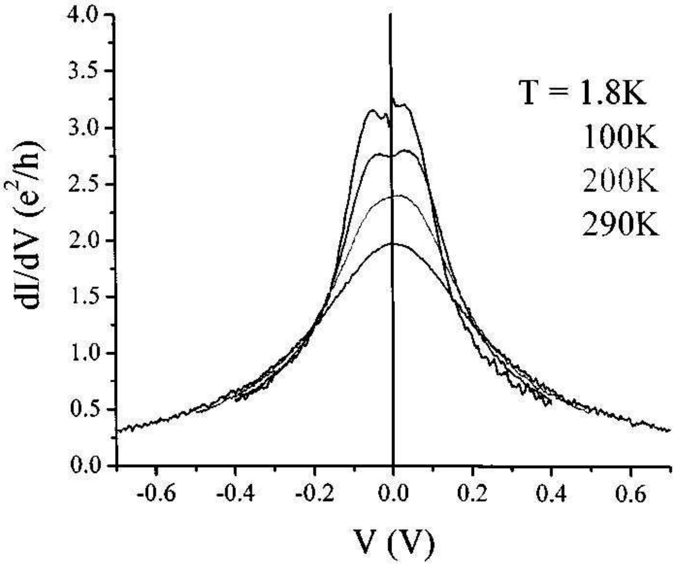

Fig. 5. *Differential conductance of a SWNT as a function of bias voltage at different temperatures.*

These results have been useful to compare the performances of the metallic CNTs with classical ohmic wires. The metallic tubes can be considered as wires with a resistance that is length-independent and diameter-independent. This is true till is valid the condition of ballistic transport, that has been experimentally demonstrated for tubes long a few micrometers [5]. For transport on longer distances or bias voltages not low enough, scattering has to be taken into account. Several groups have tried to evaluate the scattering probabilities in metallic tubes but till now no uniform results have been obtained. However using bundles of SWNTs in parallel or MWCNTs is in principle possible to obtain interconnections with any desired resistance.

The CNTs seem able to overcome the main limit that copper wires are supposed to encounter in the next future. Indeed the ITRS roadmap foresees that vertical interconnects (vias) will not be able to stand the current density required in the next future because of the impossibility of building copper vias with the same almost perfect structure of horizontal wiring [1]. Viceversa, CNTs are able to carry currents that largely satisfy the ITRS parameters till 2018. Moreover, using methods of CNTs growth in the holes between the metal layers, low resistance vias can be realized quite easily (fig. 6).

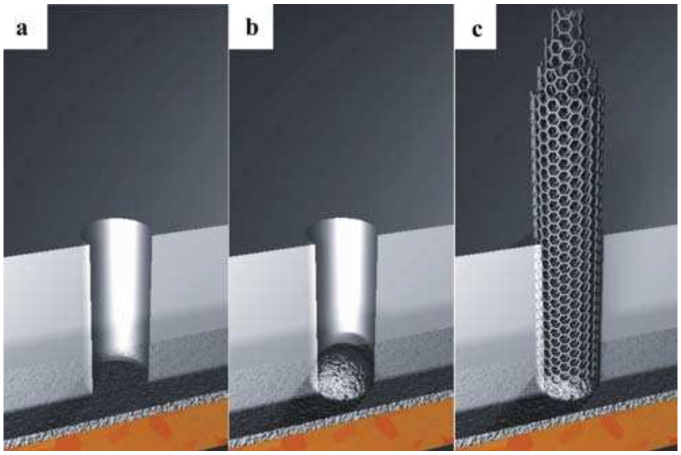

Fig. 6. *SEM image of the growth of a CNT via.*

IV. CARBONANOTUBES TRANSISTORS

The first CNT Field Effect Transistor was built in 1998 from Tans, Verschueren, and Dekker [8]. The CNT constitutes the canal of the FET, as it is shown in fig. 7.

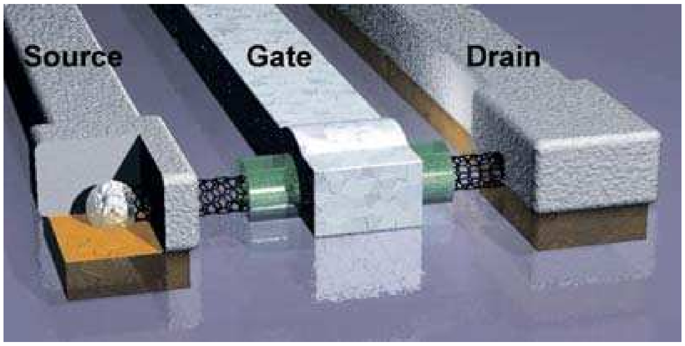

Fig. 7. *Schematic structure of a top-gated CNT Field Effect Transistor: the CNT is the canal of the transistor.*

The first CNTFET was back-gated and the drain and source electrodes were made of Potassium. The CNT used in the transistor is a semiconducting SWNT that can be switched from metallic to insulating state by the modulation of the gate voltage. This FET showed naturally a behavior similar to a p-type MOSFET. In fig. 8 the $I(V_{bias})$ curves for different gate voltages are shown. Considering the region of low bias voltages (the region in which should be polarized the future nanoelectronic devices), for positive gate voltages the current is almost totally suppressed while for negative gate voltages the conductance value saturates around $10^{-6}\ S$. In other words, the nanotube increases his conductance for negative values of the gate voltage, as shown in the inset of fig. 8. It can be noticed that, swapping the gate voltage, the conductance value can be varied over six orders of magnitude, a very satisfying range.

In this first CNTFET the saturation value of the resistance, around $1\ M\Omega$, was attributed mainly to the contact resistances between the CNT and the electrodes. However, it was not completely clear what was the reason and how were generated these high contact resistances. Almost contemporarily with the previous group, also Martel et al. [9] built and tested CNTFETs obtaining again interesting results.

After these first promising experiments, many groups built and tested their CNTFETs with CNTs produced in several ways and with different gate and electrode metals. Later on, n-type CNTFETs were obtained from a originally p-type CNTFET by doping with potassium or by simple annealing in vacuum (fig. 9). This discover made possible the realization of complementary logic, a fundamental feature for the feasibility of a digital low-power electronic made entirely of CNT devices [10].

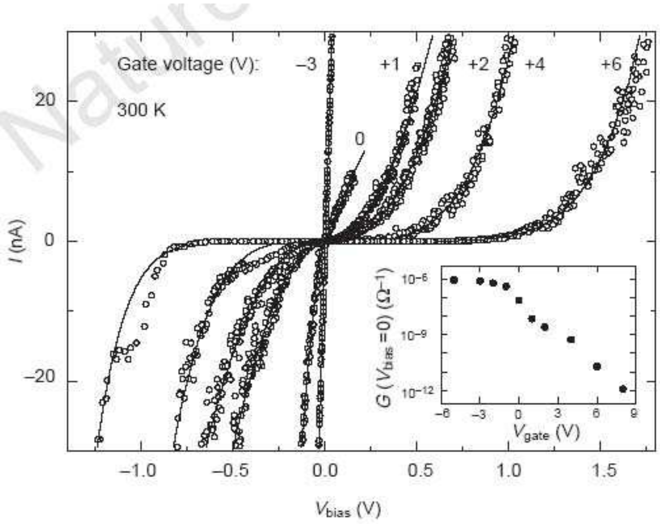

Fig. 8. *$I(V_{bias})$ curves for different gate voltages; inset, conductance of the CNT for different values of V_{gate}.*

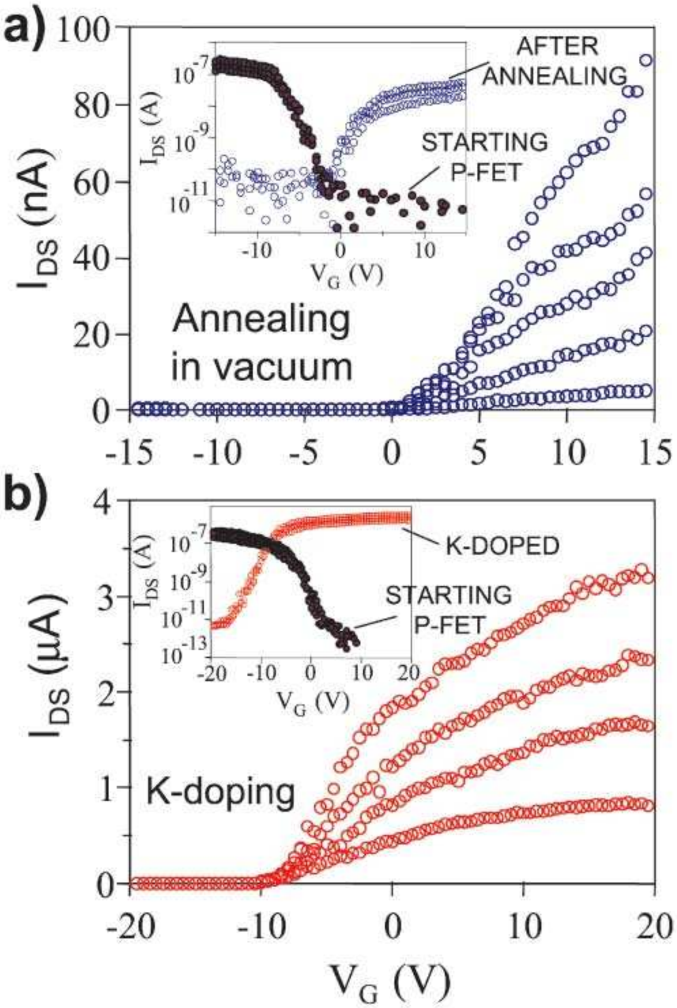

Fig. 9. *Inversion of the conductivity type of a semiconducting CNT by (a) annealing in vacuum and (b) doping with potassium. The different curves are obtained at different values of V_{DS} starting at $200\ mV$ and with increasing steps of $200\ mV$.*

However, despite of all these good results, it was not clear yet why the behavior and the performances of the CNTFETs where so heterogeneous in quite similar experiments and moreover, in some cases, not as good as expected. A very important discover was achieved when different groups showed that the transistor behavior of most of the CNTFETs built and tested till then was not due to change of the conductance of the CNT, as was believed by most of the researchers, but primarily to the variation of the drain-CNT and source-CNT contact resistances [11][12]. This effect was attributed to the Schottky barriers that are present in every semiconducting-metal junction (in this case both CNT-electrode contacts). It was shown that, changing the gate voltage, the width of these barriers was changing favoring or not the tunneling of electric charge from the contacts to the CNT and viceversa. Thus, it was mainly this phenomenon that provided the transistor-like behavior of CNTFETs and not the tube in itself!

Later on, very useful and rigorous theoretical descriptions of the electrostatic behavior and of the energy band diagrams in CNTFETs were provided by Guo et al. [13], [14] and by Castro et al. [15], [16]. Using tight analytical and numerical calculations to solve Poisson's equation, they obtained a very accurate and satisfying electrostatic analysis for the Metal-Insulator-SemiconductingCNT capacitor (in analogy with the classic MOS capacitor) and for the CNTFET in presence of various gate dielectrics and using various geometries of the capacitor and of the contacts (fig.10).

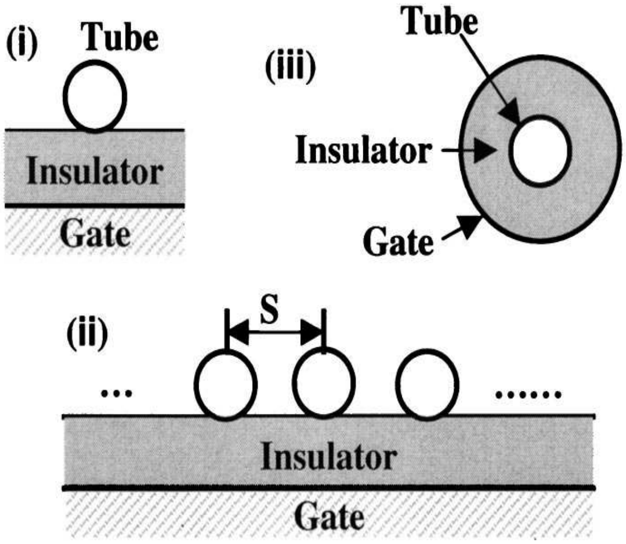

Fig. 10. *Different geometries for Metal-Insulator-SemiconductingCNT capacitor: (i) planar; (ii) periodic array; (iii) coaxial.*

These theoretical approaches shed light on the relation between the performances of the CNTFETs and the features of the electrodes of the device. In particular, it was realized that the choice of the electrode metals and of the geometry of the contacts is a basic topic in order to realize CNTFETs with good performances. Indeed, Heinze et al. [17] built a CNTFET with asymmetric contacts obtaining improvements of the performances. Moreover, Javey et al. [18] obtained a *ballistic transistor* through considerations about the work functions of the various metals used for the electrodes. Indeed, they showed that contacting semiconducting SWNTs with palladium electrodes, a metal with a high work function, strongly reduces or eliminates the Schottky barriers formed at the contacts. In this way they were able to fully exploit the ballistic properties of the CNT obtaining a CNTFET with high mobility and high current densities in low bias voltage working regions.

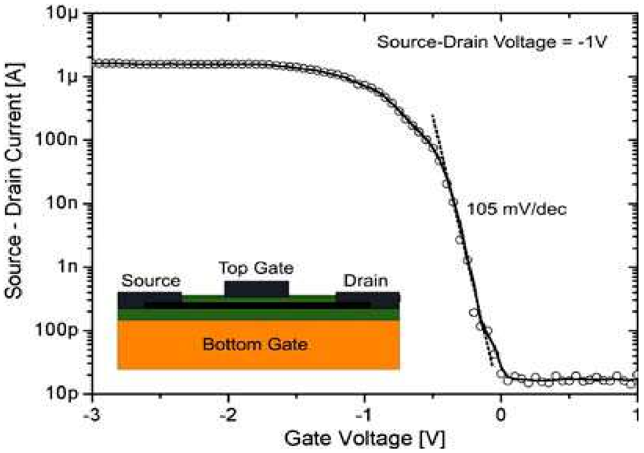

Fig. 11. *Gate voltage dependence of the source-drain current of a top-gated p-type CNTFET.*

Nowadays much research is still going on, the performances are getting better and better and the interest around CNTFETs is increasing more and more. For example Javey et al. showed that, using very short CNTs (with lengths till $10\ nm$), FETs with very high drive currents can be obtained [19]. This demonstrates that the shorter is the CNT, the lower is the probability of scattering (in other words, some kind of undercutting of the mean free path of the charges can be performed). Thus, higher bias voltages can be used and higher currents will be carried by the CNT. Furthermore, using self alignment techniques and arrays of parallel nanotubes, the performances of the CNTFETs can be further improved [20].

The CNTFETs reported in the recent literature show such good performances that they appear clearly superior to the their silicon based counterparts. In Fig. 11 it is shown the gate voltage dependence of the source-drain current of the CNTFET realized and tested recently by Seidel et al. [21]. The subthreshold slope is around $105\ mV/dec$, the on-off current ratio is around 10^5 and the saturation current is about $1.6\ \mu A$. Table I shows a comparison between the performances of the state-of-the-art Silicon transistors and this CNTFET.
From these last results, it can be realized how promising are the CNTFETs for the future of electronic devices.

V. FUTURE DEVICES

The cylindrical geometry of the CNTs inspires naturally devices with geometries that are different from planar geometries used till now in Silicon based technology. Hoenlein et al. [22] proposed recently the vertical carbonanotube FET that consists of a combination of a CNT via with a horizontal CNTFET (fig. 12a).

	CNT FET Seidel (2004)	TriGate Doyle (2003)	FinFET Yu (2002)	SON Harrison (2003)
Channel Material	CNT	Si	Si	Si
Drive Voltage $[V]$	1.0	1.3	1.2	0.9
Drive Current $[mA/\mu m]$	2.4-6.4	0.88	0.72	0.914
Transconductance $[\mu S/\mu m]$	2640-6430	920	900	1170
Subthreshold Slope $[mV/dec]$	105	69.5	101	70
On Resistance $[\Omega/\mu m]$	155-425	1480	1667	985
Gate Length $[nm]$	600	60	10	70
Gate Oxide Thickness $[nm]$	8	1.5	1.7	2
Off Current $[nA/\mu m]$	22	120	20	1

TABLE I

Comparison between the state-of-the-art p-type CNT and Silicon transistors; the values are scaled to the channel width or the CNT diameter.

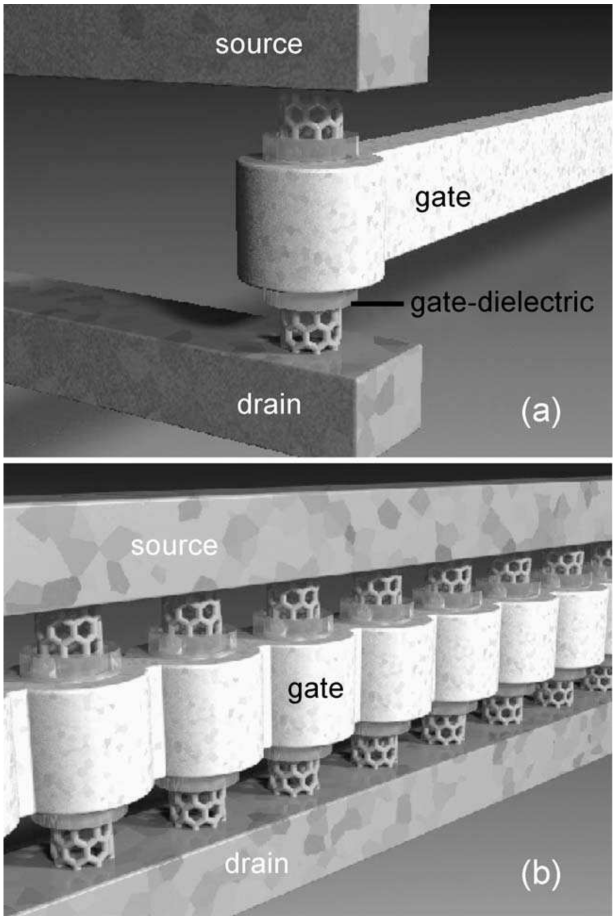

Fig. 12. *(a) Vertical CNTFET; (b) Parallel array of Vertical CNTFETs.*

This new concept opens a wide range of interesting and fascinating possibilities. Higher packing densities are allowed because source and drain areas are now on top of each other. Moreover, three-dimensional scaling of the structures can be realized because the devices are not anymore tied to the bidimensional surface of the Silicon substrate (fig. 12b).

This concept should also have in principle several advantages compared to classical planar technology in relation to the fabrication of the devices. Nevertheless, the technology of growth and treatment of CNTs is still on its infancy and still much research has to be done to make feasible these new devices.

VI. PERFORMANCE PROJECTIONS: WHAT ABOUT MODELS?

To evaluate the performances of the future CNT devices and to understand weather they can be good candidates for high performance electronic circuits, physical and circuital models are needed. In the last decade, plenty of physical models have been developed and improved [23], [24]. According to these models, CNTs devices appear in the next future to overcome the performances of the Silicon-based devices. Nevertheless, considerable steps toward reliable circuital models for circuit level simulations of systems made of CNT devices are still mostly to be done. Indeed, up to now, there are only a few models presented in literature and still in their infancy. Moreover, most of them are an extension of the classical models used for well known field-effect devices.

For instance, Dwyer et al. [25] developed a parameterizable SPICE model to evaluate the performances of future CNTFET logics. This model combines the IV characteristic of the high-performance CNTFET fabricated by Rosenblatt et al. [26] with parameterizable lumped resistances, capacitances and inductances related to the features and the various geometries of the particular technologies of fabrication under consideration.

On AC performances of CNT devices, P.J.Burke has recently performed interesting investigations [27]. For CNTs interconnections, their passive impedance is analyzed and quantified taking also into account the quantized energy levels. Through these considerations, an equivalent circuit with lumped constants is proposed. For CNTFETs, the frequency performance is analyzed taking into account typical experimental values of resistances and transconductances. A small-signal equivalent circuit is also proposed, basically derived as an extension of the one used for MOSFETs.

Through all these considerations, an estimate of the cutoff frequency of CNT devices is provided and some projections about the frequency response are made. Finally, it is claimed that in theory CNTs devices should outperform the classical silicon-based devices, although they have strong limitations mainly due to impedance mismatching with the outside world. However, these limitations should be overcame exploiting the full integration features that nanosystems should be able to provide in a further future.

VII. CONCLUSIONS

In conclusion, we provided an overview of the research running now on CarboNanoTubes devices and we described the main reasons that make them interesting candidates for future electronic devices. However, despite much research on physical level has been performed, circuital models are still to be rigorously formulated and validated.

In order to fulfill this gap, our future work will focus on the investigation of such models, attempting to take into account both the properties of quantized impedance and ballistic transport that are definitely the striking features of CarboNanoTubes.

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