Impact of Energy Band Structure on CNTFET Output Characteristics

Mariya Lyubomirova Spasova, George Vasilev Angelov, Dimitar Nikolov Nikolov and Marin Hristov Hristov

Abstract – **The electronic band structure of the nanotube is a main factor controlling the device performance of Carbon Nanotube Field Effect Transistors (CNTFETs). In this paper four different calculation models of the band structure of a zig zag carbon nanotube are used to demonstrate the influence of the electronic band structure on device characteristics. The results of calculation of the energy band structure by the different methods are then analyzed.**

Keywords – **Graphene, nanoribbon, zigzag, carbon nanotube (CNT), CNTFET, energy band structure**

I. Introduction

The semiconductor device down scaling, that follows the Moore's law, has been the main driver of technology and performance advancements in the last decades [1]. Present day conventional CMOS technologies reached the 14-nm technology node and very soon will go down to 10 nm, 7 nm and 5 nm nodes [2]. Device scaling has faced critical limitations related to fabrication technology and device performances – leakage of carriers through the thin gate oxides and leakage from source to drain, and from drain to body all due to quantum mechanical tunneling, control of dopant atoms density and location in the transistor channel as well as the source drain region, the finite sub-threshold slope and a plethora of other short-channel and narrow channel effects.

Different principal directions for finding solutions to overcome these limitations are proposed. Some of them focus on modification of existing structures and technologies to extend their scalability. Other involve the use of novel materials and technologies to replace the existing bulk silicon CMOS technology.

Despite all the limitations and challenges related to deice scaling, silicon based semiconductor technology will continue to scale down. Alternatives to conventional bulk silicon transistors such as FinFETs, that allow for fabrication of nanoscaled devices, are already present in the mainstream CMOS technologies. Other modifications of the conventional technology are focused towards implementation of novel materials and structures in the transistor channel, viz. carbon nanotubes (CNTs), to obtain higher mobility in the channel.

Graphene is a promising candidate for implementation in the future electronic devices in order to significantly boost their performance [3]. Concerning its structure, the graphene is a hexagonal monolayer sheet carbon atoms that form a 2D hexagonal lattice similar to a honeycomb. A graphene nanoribbon is called any strip that is cut out of the graphene sheet (Fig. 1). Alternatively, a nanoribbon can be thought of as an unzipped carbon nanotube (which in fact is one of the ways of nanotube fabrication).

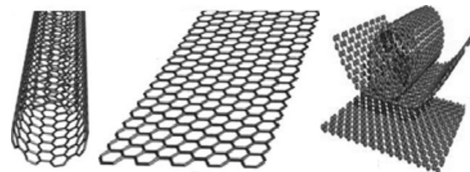

Fig. 1. Structure of single-walled CNT (*left*) and monolayer graphene nanoribbon (*middle*), and its formation (*right*).

Graphene nanoribbons are obtained by patterning a graphene sheet into strips. The boundaries of the strip (nanoribbon) can have either zigzag, or armchair, or chiral (irregular) shape [4], [5] (Fig. 2).

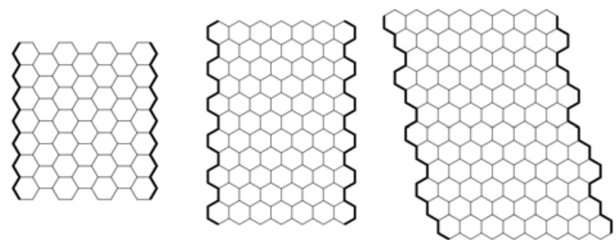

Fig. 2. Structure of a zigzag (*left*), armchair (*middle*), and chiral (*right*) graphene nanoribbon.

From energy band structure point of view, graphene is a semiconductor with zero band-gap. This is not suitable for electronic devices because in order to operate they need a band gap. For this reason, nanoribbons attract special interest as they allow to have a band gap. Combinations of monolayer and bilayer junctions are assumed to be used as switches by applying a gate voltage.

In this paper we examine four different models of band structure of 3 zigzag nanotubes: semiconducting (19,0), metallic (15,0) and semiconducting (13,0) nanotubes.

M. Spasova is with the Department of Microelectronics, Faculty of Electronic Engineering and Technologies, Technical University of Sofia, 8 Kl. Ohridski blvd., Sofia, Bulgaria.
e-mail: mls@ecad.tu-sofia.bg
G. Angelov is with the Department of Microelectronics, Faculty of Electronic Engineering and Technologies, Technical University of Sofia, 8 Kl. Ohridski blvd., Sofia, Bulgaria.
e-mail: angelov@ecad.tu-sofia.bg
D. Nikolov is with the Department of Electronics, Faculty of Electronic Engineering and Technologies, Technical University of Sofia, 8 Kl. Ohridski blvd., Sofia, Bulgaria.
e-mail: d_nikolov@tu-sofia.bg
M. Hristov is with the Department of Microelectronics, Faculty of Electronic Engineering and Technologies, Technical University of Sofia, 8 Kl. Ohridski blvd., Sofia, Bulgaria.
e-mail: mhristov@ecad.tu-sofia.bg

II. CARBON NANOTUBE FETS

Carbon Nanotube Field Effect Transistor (CNTFET) implements a carbon nanotube (CNT) in the transistor channel. A single-wall CNT (SWCNT) consists of single-layer nanoribbon rolled up in as a cylinder. The relatively straightforward implementation of manufacturing process to the state-of-the-art CMOS technology makes CNTFETs a very promising alternative to conventional MOSFETs for channel lengths sizes under 10 nm [6].

An SWCNT behaves as either a conductor or a semiconductor, depending on the particular atom arrangement when forming the nanotube cylinder. The arrangement is described and defined by the chirality vector (*n, m*). Chirality of is a crucial parameter in calculation of the CNT band structure [7]. The chirality and the energy bang structure determine whether a CNT is metallic or semiconducting. There is an empirical rule to determine CNT conductivity: if $n = m$ or $n - m = 3j$, where j is an integer, the nanotube is metallic; otherwise, the nanotube is semiconducting [8]. In Table 1 we list some chiralities of different zigzag CNTs with some parameters calculated in Matlab.

TABLE 1. PARAMETERS AND CONDUCTIVITY OF ZIGZAG TYPE CNTS

Ch	Dt [nm]	Channel [nm]	Num	E_g [eV]	Conduc-tivity
(5,0)	0.391	1.23	10	2.3	semic.
(7,0)	0.548	1.72	14	1.7	semic.
(9,0)	0.704	2.21	18	1.3	metal
(10,0)	0.783	2.46	20	1.1	semic.
(13,0)	0.101	3.19	26	0.84	semic.
(15,0)	1.174	3.69	30	0.60	metal
(19,0)	1.487	4.67	38	0.58	semiv.
(26,0)	2.035	6.396	52	0.44	semic.

Although there are several types of CNTFET structure, the most common one is shown in Fig. 3. The CNTFET *I–V* characteristics are similar to the characteristics of the conventional MOSFET.

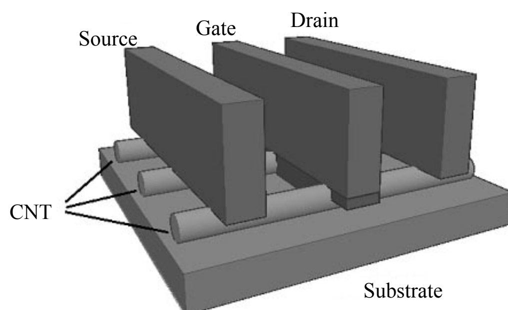

Fig. 3. Typical structure of a CNTEFT.

Two of the leading research groups on CNTFETs are at Stanford University and at IBM. The Stanford group created a carbon nanotube processor consisting of some 178 transistors. Each of them has carbon nanotubes with length between 10 to 200 nm [9], [10], [11]. The IBM Systems and Technology Group has demonstrated individual carbon nanotube transistors with channels smaller than 10 nm with better performance (faster, more energy efficient) than the silicon MOSFETs [6].

III. ENERGY BAND CALCULATION APPROACHES

The one and only complete behavioral compact model of CNTFET so far is the Stanford University CNTFET model [12], [13]. The model was released in 2008 and since then it is constantly updated by adding or refining different features [8]. The latest version of the Stanford model is Virtual-Source Carbon Nanotube FET (VS-CNFET) [14], [15]. It describes semi-empirically the *I-V* characteristics in a short-channel FET. The difference between the original Stanford CNFET model and the VS-CNFET model is in the approach of modeling the carrier transport.

There are different methods for calculation of the energy band structure (the *E-k* dispersion). The Density Functional Theory (DFT) that is based on Hohenberg-Kohn theorems [16] and the Kohn-Sham equations [17] is most frequently used. However, it requires a lot of computational resources due to its complex equations.

Tight-binding (TB) approaches for calculations of band structure are also popular for energy band calculation due to their computational efficiency and the atomistic nature of the treatment [18], [19]; in particular the orthogonal p_z tight-binding (OTB) approach has been widely used for CNTs structures calculations [20]. Slater–Koster tight-binding scheme is also employed sometimes [21].

For CNTs diameters less than 1 nm, the approach based on the Extended Hückel Theory (EHT) is usually applied [22], [23]. The main difference between a common OTB approach and EHT is that the orbital basis functions are nonorthogonal in the latter. In contrast to OTB, the EHT-basis functions are formulated explicitly which allows for easier calculation of Hamiltonian matrix elements.

We use the original Stanford CNFET model [12], [13] coded in Verilog-A to perform simulations in Cadence Spectre circuit simulator. We do several simulations, each time using a different Verilog-A code for calculation of the *E-k* dispersion relationship, and in particular we modify the perpendicular component of the energy subband in accordance with the above described different approaches for energy band structure calculation.

Afterwards, we simulate the *E-k* dispersion relationship in Matlab using the numerical approach described in [24] that is also used in the original Stanford CNFET model. In the Stanford model the Born-Karman boundary conditions on both the circumferential and axial direction are used [12].

Next we do simulations in VirtualNanoLab [25] using the above calculation approaches in order to compare the results with the results of Verilog-A and Matlab calculations.

Finally, we input back in the original Verilog-A code the results obtained by the simulations in VirtualNanoLab and Matlab. In this way, we calibrate the initial Verilog-A model.

IV. BAND STRUCTURE MODELS

The band structure of CNTs can be computed by substituting the allowed wavevectors into the energy

dispersion. NNTB energy *E-k* dispersion relation of graphene is described in Eq. (1).

$$E(k) = \pm\gamma\sqrt{1+4\cos\left(\frac{\sqrt{3}a}{2}k_x\right)\cos\left(\frac{a}{2}k_y\right)+4\cos^2\left(\frac{a}{2}k_y\right)} \quad (1)$$

where the plus and minus signs denote the conduction and valence band respectively. *Kx* and *Ky* are the vector components describing the geometry and chirality of the CNT; they are described with Eq. (2) and Eq. (3).

$$Kx = \frac{2\pi\sqrt{3}aj(n+m)Ch + a^3k(n^3-m^3)}{2Ch^3} \quad (2)$$

$$Ky = \frac{\sqrt{3}ak(n+m)Ch + 2\pi aj(n-m)}{2Ch^2} \quad (3)$$

$$k = \frac{2\pi}{NucT}l, l = 0,1,...., Nuc - l, \quad (4)$$

where *Ch* is the chiral vector, *l* is determined by the unique solution of *K*, restricted to the first Brillouin zone. *K* determines the wavevectors within the Brillouin zone that lead to the Bloch wave function. The wave vector *q* describes CNT along the circumferential direction Eq. (5).

$$q = \frac{2\pi}{Ch}j, j = 0,1,...j_{max} \quad (5)$$

The band structure of the zigzag semiconducting (19,0) nanotube is calculated using the numerical approach described in [18]. The zigzag CNT is an attractive type of nanotube because of its high symmetry. It leads to a simple analytical expression of many solid-states properties. The energy dispersion for zigzag CNTs can be obtained from the Brillouin zone wavevector (Eq. 6) [24].

$$E(j,k) = \pm\gamma\sqrt{1+4\cos\left(\frac{\sqrt{3}ka}{2}\right)\cos\left(\frac{j\pi}{n}\right)+4\cos^2\left(\frac{j\pi}{n}\right)} \quad (6)$$

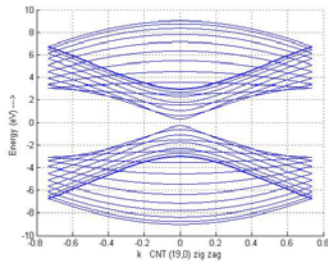

Fig. 4. Band structure of (19,0) zigzag nanotube containing 38 1D-subbands in the conducting and valence bands

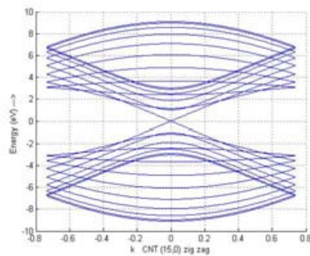

Fig. 5. Band structure of (15,0) zigzag nanotube containing 30 1D-subbands in the conducting and valence bands

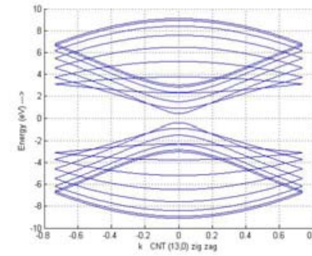

Fig. 6. Band structure of (13,0) zigzag nanotube containing 26 1D-subbands in the conducting and valence bands

In Fig. 4, 5 and 6 we show the band structure for semiconducting (19,0), metal (15,0) and semiconducting (13,0) nanotubes calculated in Matlab using the numerical approach described in [24]. The CNT diameters are 1.487 nm, 1.174 nm, and 0.101 nm respectively. In Fig. 5 the metallic CNT shows a band degeneracy at 0 eV and *k*= ±*π*/(√3a). The semiconducting (19,0) CNT has a bandgap of 0.58 eV.

Fig. 7, 8 and 9 plot the band structure of semiconducting (19,0), metal (15,0) and semiconducting (13,0) nanotubes calculated using VirtualNanoLab [25] with its band structure calculators using DFT, extended Hückel and Slater-Koster approaches.

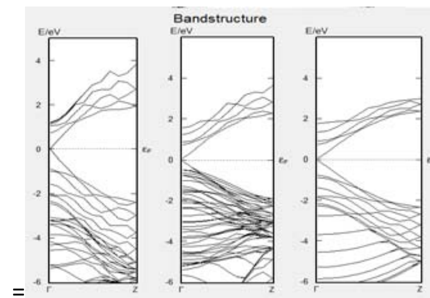

Fig. 7. Calculation using a) DFT, b) Hückel and c) Slater-Koster calculator in the semiconducting zigzag (15,0) CNT

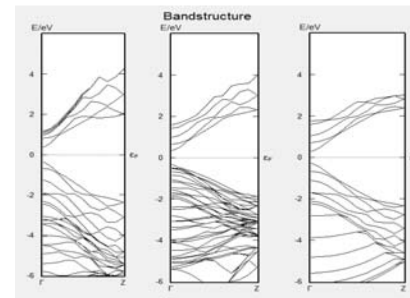

Fig. 8. Calculation using (a) DFT, (b) Hückel, and (c) Slater-Koster calculator in the semiconducting zig zag (13,0) CNT

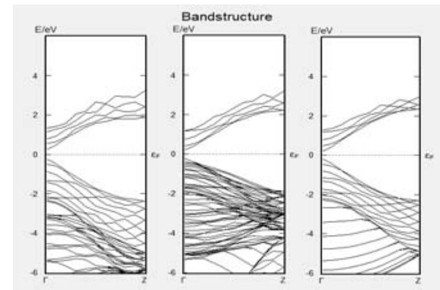

Fig. 9. Calculation using (a) DFT, (b) Hückel and (c) Slater-Koster calculator in the semiconducting zig zag (19,0) CNT

V. Simulation Results

Simulation results show a change in the energy of the first conduction zone varying between 0.2001 to 0.2236 eV. In order to estimate the impact of the first energy band on the output *I-V* characteristics of the CNTFET the simulated output characteristics are shown in Fig. 7.

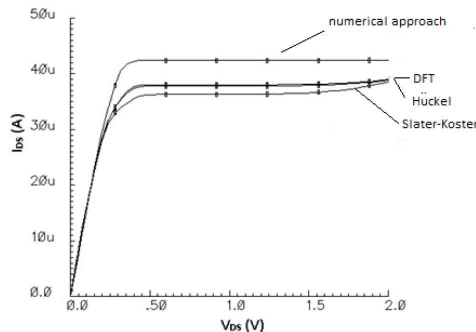

Fig. 7. I_{DS} (V_{DS}) at V_{GS} = 0.9 V results for the (19,0) CNTFET using numerical approach, DFT, Hückel and Slater-Koster calculator in CNTFET

The drain current value calculated by the numerical method is IDS = 0.42 μA. When applying the methods of DFT, extended Hückel, and Slater-Koster the drain current is IDS = 0.38 μA, 0.382 μA, and 0.3782 μA respectively.

VI. Conclusion

In this paper four different calculation models of the band structure of a zigzag (19,0) carbon nanotube has been studied using numerical, DFT, Slater-Koster and Hückel calculation approaches. We compared the results from the above mentioned approaches in Matlab and input them back in the original Verilog-A code. In result the impact of electronic band structure on device output characteristics has been demonstrated.

Acknowledgment

The research in this paper was carried out within the framework of Contract No. DUNK 01/03 dated 12.2009.

References

[1] G. Moore, Progress in Digital Electronics, *IEDM Tech Digest*, 1975, pp. 11-13.
[2] The International Technology Roadmap for Semiconductors http://www.itrs.net
[3] A. K. Geim and K. S. Novoselov, "The rise of graphene," Nat. Mater., vol. 6, no. 3, pp. 183–191, Mar. 2007.
[4] L. Jiao, L. Zhang, X. Wang, G. Diankov, H. Dai, Narrow graphene nanoribbons from carbon nanotubes, *Nature*, 458 (7240), pp. 877–880, 2009.
[5] D.V. Kosynkin, A.L. Higginbotham, A. Sinitskii, J.R. Lomeda, A. Dimiev, B.K. Price, J.M. Tour, Longitudinal unzipping of carbon nanotubes to form graphene nanoribbons, *Nature*, 458 (7240), pp. 872–876, 2009.
[6] A. Franklin, M. Han Sh.,, G. Tulevski, Ch. Breslin, L. Ginac, M. Lundstrom, W. Haensch, Sub-10 nm Carbon Nanotube Transistor, *Nano Letters*, 2012, 12 (2), pp 758 – 762.
[7] J. Mintmire and C. White, Universal Density of States for Carbon Nanotubes, *Phys. Rev. Let.*, vol. 81, pp. 2506-2509, 1998.
[8] Stanford University CNFET model Website: http://nano.stanford.edu/model.php
[9] http://www.technologyreview.com/news/511746/stanford-researchers-build-complex-circuits-made-of-carbon-nanotubes/
[10] http://www.technologyreview.com/news/519421/the-first-carbon- nanotube-computer/
[11] A. Javey, J. Guo, D. B. Farmer, Q. Wang, D. Wang, R. G. Gordon, M. Lundstrom, and H. Dai, Carbon nanotube field-effect transistors with integrated ohmic contacts and high-k gate dielectrics, *Nano Letters*, vol. 4, no. 3, pp. 447–450, 2004.
[12] J. Deng and H.-S. P.Wong, A compact SPICE model for carbon nanotube field effect transistors including non-idealities and its application—Part I: Model of the intrinsic channel region, *IEEE Trans. Elec. Devices*, vol. 54, no. 12, pp. 3186–3194, 2007.
[13] J. Deng and H.-S. P.Wong, A compact SPICE model for carbon nanotube field effect transistors including non-idealities and its application—Part II: Full Device Model and Circuit Performance Benchmarking, *IEEE Trans. Electron Devices*, vol. 54, no. 12, pp. 3195–3205, 2007.
[14] C.-S. Lee, E. Pop, A. Franklin, W. Haensch, and H.-S. P. Wong, A Compact Virtual-Source Model for Carbon Nanotube Field-Effect Transistors in the Sub-10-nm Regime—Part I: Intrinsic Elements, arXiv: preprint1503.04397 .
[15] C.-S. Lee, E. Pop, A. Franklin, W. Haensch, and H.-S. P. Wong, A Compact Virtual-Source Model for Carbon Nanotube Field-Effect Transistors in the Sub-10-nm Regime—Part II: Extrinsic Elements and Performance Assessment, arXiv: preprint1503.04398
[16] Pierre Hohenberg and Walter Kohn. Inhomogeneous electron gas. *Physical review*, 136(3B):B864, 1964.
[17] Walter Kohn and Lu Jeu Sham. Self-consistent equations including exchange and correlation effects. *Physical Review*, 140(4A):A1133, 1965.
[18] P. Vogl, H. P. Hjalmarson, and J. D. Dow, "A semi-empirical tightbinding theory of the electronic structure of semiconductors," *J. Phys. Chem. Solids*, vol. 44, no. 5, pp. 365–378, 1983.
[19] T. B. Boykin, G. Klimeck, and F. Oyafuso, "Valence band effectivemass expressions in the sp d s empirical tight-binding model applied to a Si and Ge parametrization," *Phys. Rev. B*, vol. 69, p. 115201, 2004.
[20] R. Saito, G. Dresselhaus, M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes*. UK Imperial College Press, 2003
[21] J. C. Slater and G. F.Koster, "Simplified LCAOmethod for the periodic potential problem," *Phys. Rev.*, vol. 94, pp. 1498–1524, Jun. 1954.
[22] J. N. Murrell and A. J. Harget, *Semi-Empirical Self-Consistent Molecular Orbital Theory of Molecules*. New York: Wiley Interscience, 1972.
[23] D. Kienle, J. I. Cerda, and A. W. Ghosh, "Extended Hückel theory for electronic structure, chemistry and transport. I. Carbon nanotubes," *J. Appl. Phys.*, accepted for publication.
[24] H. Wong, and D. Akinwande, *Carbon Nanotube and Graphene Device Physics*, Cambridge University Press (2010).
[25] VirtualNanoLab website: http://quantumwise.com/products/vnl