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BAND STRUCTURE OF CNT EFFECT ON THE CNTFET PERFORMANCES

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ABSTRACT

Carbon nanotubes (CNT) has been seen as a potentially future material to provide an ultra small device by their exceptional electronic, optical, thermal, and mechanical properties, make them a promising candidate for applications in micro and nanoelectronics (essential in an application type transistor CNTFET (Carbon Nanotube Field Effect Transistor)). Using the available models, we simulated and analyzed the influence of the band structure of carbon nanotube on the device characteristics. Also in this paper, We present analytical modelling of the effective densities of states for the conduction and valence bands of a zigzag single-walled semiconducting carbon nanotube field effect transistor (CNFET) using the dispersion relation E(k) (the three first sub band) of the band structure of the carbon nanotube can be obtained by zone-folding approximation. In order to show the influence of the three first sub-band energy on DOS (Density Of State) of CNTFET.

KEYWORDS: Band Structure, Carbon Nanotube, Density of State, CNTFET, Zone Folding

INTRODUCTION

The nanotechnologies represent a domain of the scientific research and the rapidly growing industry. This extremely fast development however implies the potential exhibition in manufactured nanomaterials dune more important population, for the workers in industrial environment and in research laboratories (Joshua and Andrew, 2009).

Carbon nanotubes CNT are a new modification of carbon discovered in 1991 by Ijiima while looking at soot residues from a fullerene experiment. Carbon nanotubes are high aspect ratio hollow cylinders with diameters ranging from one to tens of nanometers, and with lengths up to several micrometers. CNTs are hollow cylinders composed of one or more concentric layers of carbon atoms in a honeycomb lattice arrangement (Appenzeller *et al,* 2002; Ijiima *et al,* 1991). It can be classified into SWCNT (Single Walled Carbon Nano Tube) and MWCNT (Multi Walled Carbon Nano Tube Both types are attractive for nanoelectronic applications of future, either as active element, or as interconnection element., this raises the scope for new integrated circuit technologies made from CNT transistors and interconnects (Philipwong *et al,* 2011; Avouris *et al,* 1999; Martel *et al,* 1998). Semiconductor CNT can be used as active elements in field-effects transistors (CNTFETs). Since the first experimental demonstrations in 1998, the performances of these components did not stop improving. Intensive searches are in progress to develop the adapted technologies and estimate the static and dynamic characteristics of transistors at nanotube of carbon (CNTFET) (Prabhakar 2007; Alvi *et al,* 2005). In this work using the zone folding approximation for determined the dispersion Energy E(k), we simulated the band structure of CNT with the three first sub band. We studied also the influence of the three first sub-band energy on DOS (density of state) of CNTFET.

ELECTRONIC BAND STRUCTURE OF CNT

The structure of a CNT can be seen as the result of the rolling up of a graphene sheet with the width defined by a lattice vector $\vec{C}_h$ "Figure 1". The rolling up is geometrically characterized by the indices n and m which specify the

diameter and the helicity angle of the CNT and determine its fundamental properties (Philipwong *et al*, 2011; Upasani *et al*, 2010; Nizam *et al*, 2010).

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

where $\vec{a}_1 = a\left(\sqrt{3}/2, 1/2\right)$ and $\vec{a}_2 = a\left(\sqrt{3}/2, -1/2\right)$

a =0.142nm, (is the distance between two carbon atoms). The magnitude of $\vec{C}_h$ corresponds to the circumference around the nanotube. This can be used to determine the diameter (d) as denoted by:

$$d_t = \left(\sqrt{3}a_{CC}\sqrt{m^2 + mn + n^2}\right)/\pi \tag{2}$$

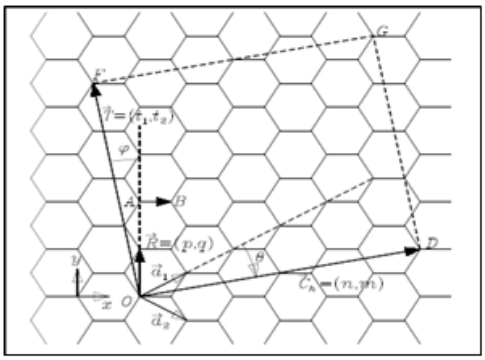

Figure 1: Circumferential Vector $\vec{C}_h$ and Vector $\vec{T}$ in Real Space Graphene Lattice (Philipwong et al, 2011)

The rolled-up nanotube is a one-dimensional periodic structure with a unit cell which is a rectangle defined by the chirality's vector $\vec{C}_h$ and the primitive translation $\vec{T}$. The 2D Brillion zone of the nanotube unit cell is a rectangle in the reciprocal space defined by the vectors $\vec{C}_h$ and $\vec{T}$. Where:

$$\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2 \tag{3}$$

Since the condition $\vec{C}_h . \vec{T} = 0$ must be satisfied, t_1 and t_2 can be expressed in terms of m and n (Nizam *et al*, 2010).

where: $t_1 = \dfrac{2m+n}{N}$ and $t_2 = -\dfrac{2n+m}{N}$

As we shall see, the way of rolling is extremely important for the nanotube properties. The values of the electron wave vector in a nanotube k are restricted additionally by the rotational boundary condition $k . \vec{C}_h = 2\pi q$.

Where q = 0, 1, 2, …, N-1, N is the number of carbon pairs in the unit cell (Charlier *et al*, 2007; Xinghui *et al*, 2004).

$$\mathrm{N} = 2 \cdot \left(n^2 + m^2 + nm\right)/d_R \tag{4}$$

with : d_R=gcd (2m+n, 2n+m).

Therefore, the allowed values of k lie on N equidistant lines parallel to the tube axis "Figure 2".

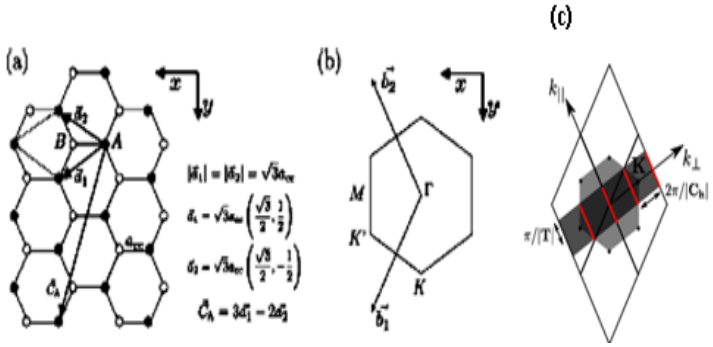

Figure 2: Brillion Zone and Reciprocal Space, (a) Basis Vector in the Hexagonal Lattice of Graphene, (b) Brillion Zone Corresponding Reciprocal Basis Vector b_1 and b_2, (c) the Allowed Values of k Lie on N Equidistant Lines Parallel to the Tube Axis (Charlier et al, 2007)

The one-dimensional (1D) band structure of a *(n, m)* nanotube is given by the zone-folding relation by use of the two-dimensional band structure of grapheme (Popov *et al*, 2004; Lia *et al*, 2006).

$$E_{NT}(k,q) = E_{2D}\left(k\frac{K_2}{|K_2|} + qK_1\right) \tag{5}$$

$$K_1 = \frac{-t_2 b_1 + t_2 b_2}{N} \text{ and } K_2 = \frac{mb_1 - nb_2}{N}$$

where: b1= b(1/ 2, 3 / 2) and b_2=b(1/ 2,− 3 / 2) , b= 4π/3acc

E_{2D} is The E-k values for 2D graphene structure .The zone-folding method gives reasonable predictions for the band structure and the optical transition energies for radii, larger than about 6 Å (Popov and Henrard, 2004).

MODEL EQUATION OF THE DENSITY OF STATE (DOS)

The density of state (DOS) obtained by diversion of this one presents peaks called peculiarities of van Hove (SvH) below (and top) of every sub-band. Furthermore, in the case of the linear bands, the density of state is constant (Mintmire and White, 1998). The DOS equation can be obtained by substituting the equation of $dk = \frac{2\pi dN}{L_X}$ for the derivation of the band structure equation given by the zone folding (10). Note that the used equation to reorganize the equation (10) in terms of *k* and to simplify for product the following equation:

$$k = \sqrt{\frac{4\beta^2}{E_G}\left(E - \frac{E_G}{2}\right)} \tag{6}$$

$$\beta = \left(\frac{2}{d_t}\right)^2 \cdot \left(q \pm \frac{\alpha}{3}\right)^2 \tag{7}$$

$$E_g = \frac{\sqrt{3}a\gamma_0}{2\beta} \tag{8}$$

Le résultat DOS équation était:

$$DOS(E) = \frac{dN}{L_X dE} = \frac{\beta}{2\pi\sqrt{E_g}}\left(E - \frac{E_g}{2}\right)^{-\frac{1}{2}} \quad (9)$$

β used in equation (9) is pulled the equation (10) which consists the equation sub-band, It means, every sub-band will have their own value of β, what allows the simulation of DOS(E) for various sub-bands.

RESULTS AND DISCUSSIONS

The band structure consists of valence band, band gap and conduction band. Both valence band and conduction band will split into first, second and third sub-bands. Band structure modeling only can be simulated when energy-wave vector E (k) dispersion equation is found. However, the E (k) dispersion equation must relate to the first, second and third sub-band in order to determine the position of sub-band in a band structure (Popov and Henrard, 2004). The E (k) dispersion relation can be expressed as:

$$E_q^{\pm}(k_{II}) \cong \pm\frac{\sqrt{3}a\gamma_0}{2}\cdot\sqrt{\left(\frac{2\pi}{|C|}\right)^2\cdot\left(q\pm\frac{1}{3}\right)^2 + {k_{II}}^2} \quad (10)$$

$$\Delta E_g = E^+_{q=0}(k=0) - E^-_{q=0}(k=0) = \frac{2\pi a\gamma_0}{|C|} = \frac{2a\gamma_0}{d_t} \quad (11)$$

Where ΔEg is the band gap energy, dt is the tube diameter, γ_0 is the energy between carbon atom, where a is the lattice constant of the honeycomb network, a =0.142nm, (is the distance between two carbon atoms) the integer variable q counts the available bands, whereas k is the part of the wave vector that continuously describes the states within a given sub-band (and associated with the direction parallel to the tube axis).

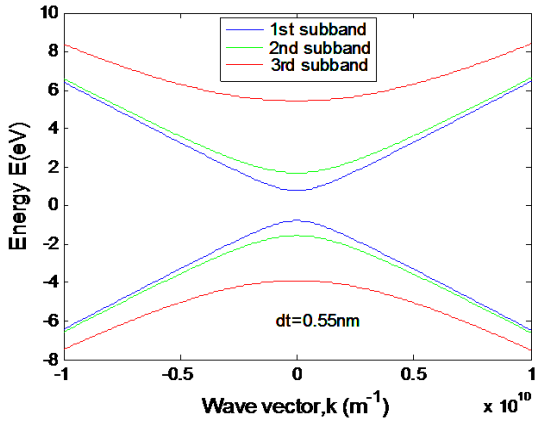

Figure 3: The E (k) Dispersion Energy with CNT Sub-Band

Show in "Figure 3" the graphs of E (k) dispersion based on the equation (10) which is valid near k=0, and these curve are plotted for several sub-bands. Based on the simulation, the first sub-band has smaller band gap, followed by second sub-band and the third sub-band which has the biggest band gap.

This indicates that the carriers in the first sub-band are easier to move from valence to conduction band due to the smaller band gap compared to the other sub-bands.

The density of the States of SWCNT, such as discussed previously is given by the expression (9), we simulated the first sub-band presented the "Figure 4";

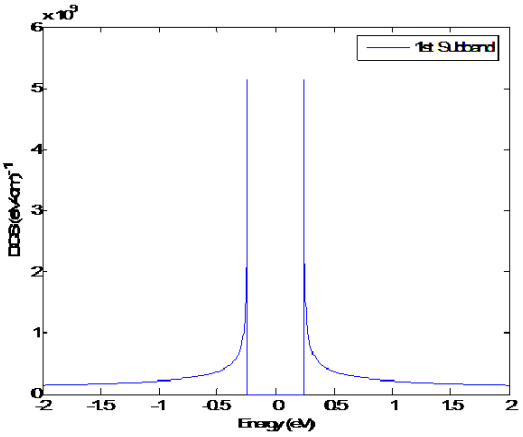

Figure 4: Densité d'Etat Pour La Première Sous Bande

When we drew the variation of dispersion of energy ' E (k) ', the Density of States of Nanotube DOS (E) varies as accordingly like in the "Figure 4". We can observe a symmetric density of states around the level of Fermi with the maximum and the minimum just over the band of conduction and just below the band of valiancy respectively. The DOS is simulated for three sub-bands on the "Figure 5". Note that the simulation is only for the semiconductor of type zigzag *(n, 0)*.

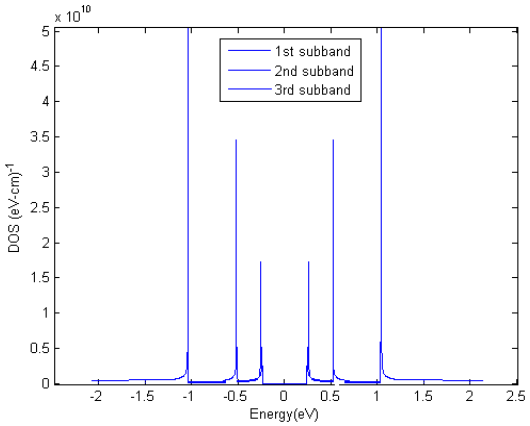

Figure 5: Density of State for the Three First Sub-Bands

The simulation above shows the density of state according to the energy. This simulation includes the first, second and third sub-bands. As we already knew, zero available states between the band of conduction and the band of valence shown that a substantial distance from band exists in the CNT. This distance is good express by the result of simulation of band of energy E (k).

The level of energy which can occupy by states in the first sub-band is smaller than in second and third sub-bands. This is because the DOS is proportional in the energy and because the first sub-band on the smaller of dispersal energy compared with the higher sub-band, so the DOS is also the smallest among three sub-bands.

CONCLUSIONS

From a model of CNTFET, we have implemented a physical based calculation of the sub-bands energy. This calculation, obtained from a zone-folding method, the analysis of the related simulated the dispersion of energy E(k) for the three first sub-bands has shown that the CNT sub-bands have a significant impact on the DOS and the band gap . The first sub-band has important effect in the CNTFET characteristic compared with the second and third sub-band.Les

résultats du modèle sont comparés avec ceux obtenus par des résultats expérimentaux donnés par la littérature, par le biais des courbes résultantes de la simulation effectuée en MATLAB 7.4.

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