Analysis of Electronic Structure of Carbon Nanotubes

Mariya Spasova, George Angelov, Anna Andonova, Tihomir Takov, and Marin Hristov

Abstract – Single-walled carbon nanotube provide huge potential for the carbon-based nanodevices and circuit integration. This paper focuses upon the study of single-walled carbon nanotubes with zig zag (3,0) chirality, armchair (3,3) chirality, and Chiral (3,2) chirality. Bloch States, transmission spectrum, density of States, and band structure of Carbon nanotubes are simulated in Virtual Nanolab simulator and validated against experimental measurements of the CNT structure.

Keywords - CNTFET, chirality, band structure, graphene.

I. Introduction

Single-Walled Carbon Nanotubes (SWNTs) are members of the carbon family of fullerenes. Their unique structure and nanometer sizes which are promising for nanoelectronic and nanomechanical applications [1]. The geometry of the Carbon Nanotubes is that of a hollow cylinder. The carbon atoms are arranged in a honeycomb crystalline lattice. The atomic structure of a single-walled carbon nanotube is described by its chiral indices (n, m).

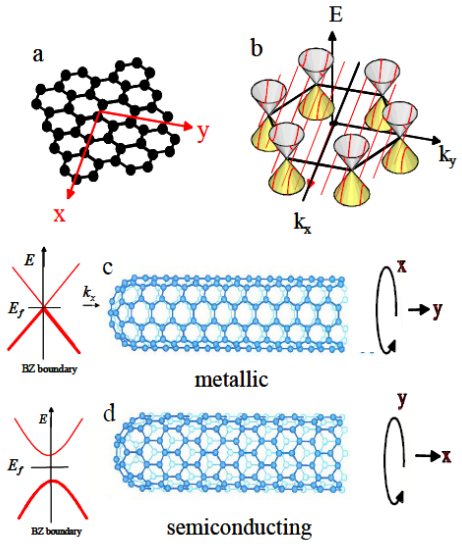

Fig. 1. (a) The lattice structure of graphene, a honeycomb lattice of carbon atoms. (b) The energy of the conducting states as function of the electron wavevector k. (c), (d) Graphene sheets rolled into tubes. This quantizes the allowed k's around the circumferential direction, resulting in 1D slices through the 2D band structure in (b). Depending on the way the tube is rolled up, the result can be either a metal (c) or a semiconductor (d) [2].

Graphene consists of a 2D honeycomb structure of sp^2 bonded carbon atoms as shown in Fig. 1(a). Its band structure has conducting states at *Ef*, but only at specific points along certain directions in momentum space at the corners of the Brillouin zone as shown in Fig. 1(b). The momentum of the electrons moving around the circumference of the tube is quantized. This quantization results in tubes that are either one-dimensional metals or semiconductors, depending on how the allowed momentum states compare to the preferred directions for conduction. Choosing the tube axis to point in one of the metallic directions results in a tube whose dispersion is a slice through the center of a cone (Fig. 1(c)). The tube acts as a 1D metal with a Fermi velocity υ_f = 8 x 10^5 m/s comparable to typical metals. If the axis is chosen differently, the allowed *k*s take a different conic section, such as the one shown in Fig 1(d) [2].

In this paper are described single-walled carbon nanotubes with different chirality. In paragraph II are calculated a several possible parameters of the tubes with different chirality. Section III describes the results of analysis of Carbon nanotubes with zig zag (3,0) chirality, armchaire (3,3) chirality, and Chiral (3,2) chirality. Bloch States, transmission spectrum, density of States, and band structure of Carbon nanotubes are simulated in Virtual Nanolab simulator.

II. Theoretical Calculation of SWNTs

A. Structural description of carbon nanotubes

We are using the solid state physics convention to describe the graphene lattice structure, where the basis vectors of the graphene net $\vec{a}_1$ and $\vec{a}_2$ ($a_1 = a_2 = a_o$ = 0.246 nm) are separated with an inter-angle of 60°, as shown schematically in Fig. 2 in radial projection. The diameter, *d*, of the carbon nanotube is

$$d = \frac{a_0}{\pi}\sqrt{n^2 + nm + m^2} \qquad (1)$$

and the helicity, α, defined as the angle between the perimeter vector, $\vec{A} = (n, m)$, and the basis vector, $\vec{a}_1$, illustrated in Fig. 2 , is

$$\alpha = \tan^{-1}\left(\frac{\sqrt{3}m}{2n + m}\right) \qquad (2)$$

The chiral indices (n_c,m_c), perpendicular to the chiral

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vector, $\vec{A}$, can be calculated by orthogonallity relationship between the tubule perimeter and the tubule axis

$$\frac{m_c}{n_c} = -\frac{2n+m}{n+2m} \tag{3}$$

The axial periodicity, *c*, of Carbon nanotube (*n, m*) can be obtained

$$c = a_0\sqrt{n_c^2 + m_c^2 + n_c m_c} \tag{4}$$

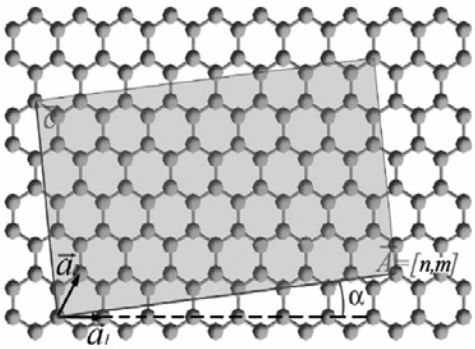

Fig. 2. Schematic structure of graphene with basis vectors $\vec{a}_1$ and $\vec{a}_2$. The shadowed rectangle is the radial projection of carbon nanotube (7,1) with perimeter $\vec{A}$ and helical angle α [3].

The atomic positions of a single-walled carbon nanotube can be conveniently expressed by the Cartesian coordinates (x_j, z_j) in the radial projection, where the nanotube is projected onto a rectangle with sides *A* and *c* as described above [3].

B. Calculation results

In this paragraph are calculated a several possible parameters of the tubes with different chirality, as listed in Table 1. The table lists the some types of chirality of zig zag, armchair, and chiral tubes with fixed bond length □$_0$ = 2.46 [Å].

TABLE I
LIST OF CHIRAL INDICES (n, m), DIAMETER (d), AND HELICITY (α) OF CARBON NANOTUBES

	Chirality (*n, m*)	□$_1$ [Å]	□$_2$ [Å]	*d* [Å]	*α* [°]	□$_0$ [Å]
zig zig	(3, 0)	1.6735	1.6735	2.35	0	2.46
	(6, 0)	1.6735	1.6735	4.70	0	2.46
	(9, 0)	1.6735	1.6735	7.05	0	2.46
	(18, 0)	1.6735	1.6735	14.10	0	2.46
armchair	(3, 3)	1.6735	1.6735	7.046	30	2.46
	(6, 6)	1.6735	1.6735	8.141	30	2.46
	(9, 9)	1.6735	1.6735	12.21	30	2.46
	(10, 10)	1.6735	1.6735	13.56	30	2.46
Chiral	(3, 2)	1.6735	1.6735	3.414	23.413	2.46
	(6, 4)	1.6735	1.6735	6.829	23.413	2.46
	(9, 8)	1.6735	1.6735	11.54	28.054	2.46

III. SIMULATIONS

In this paragraph are simulated Carbon nanotubes with chirality (3,0), (3,3), (3,2) in Virtual Nanolab simulator. In Fig. 3 are shown the bulk configurations of carbon nanotubes with the mentioned chirality.

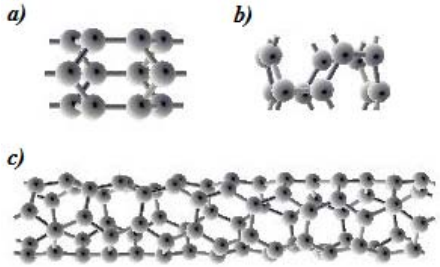

Fig. 3. Bulk configuration - a) (3,0), b) (3,3), c) (3,2).

In Fig. 4, 5, and 6 Bloch States of carbon nanotubes with the above mentioned chirality are shown. Bloch states can be used to investigate the symmetry of certain bands. This can be related to the transport properties of Carbon nanotubes. In Fig. 5 the full symmetry is shown between "up" and "down" spin states. In Fig. 4 the tube with chirality (3, 3) shows lower bond strength than Carbon nanotubes with chirality (3, 0). In Fig. 6 the tubes are Chiral type and they have full symmetry.

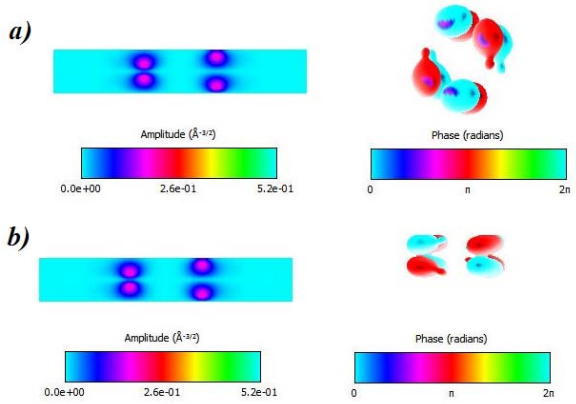

Fig. 4. Bloch States of Carbon nanotubes with chirality (3,3) - a) „up" spin orientation and b) „down" spin orientation

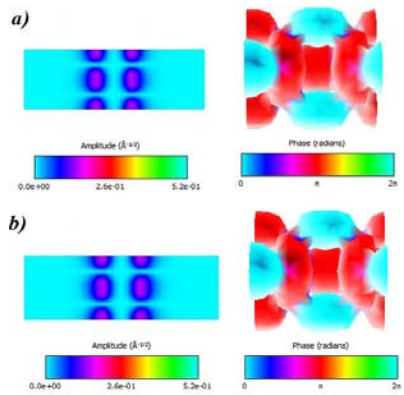

Fig. 5. Bloch States of Carbon nanotubes with chirality (3,0) – a) „up" spin orientation and b) „down" spin orientation

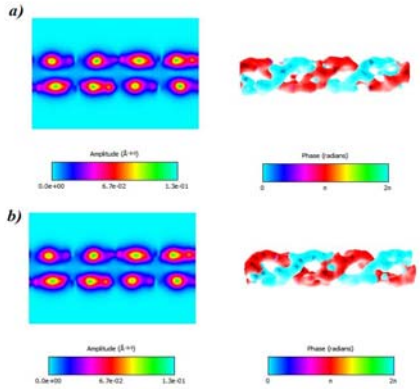

Fig. 6. Bloch States of Carbon nanotubes with chirality (3,2) - a) „up" spin orientation and b) „down" spin orientation

In Fig. 7, 8, and 9 Density of States of carbon nanotubes with the same (3,0), (3,3), (3,2) chirality are shown. Density of States of carbon nanotubes shows the energy gap around the Fermi level. This can be seen in Fig. 7 and 8. In Fig. 9 we do no observe energy gaps because the tube with chirality (3,2) is of Chiral type.

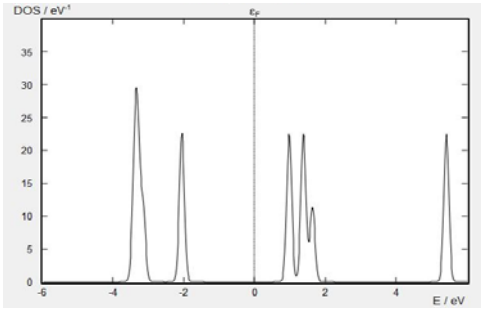

Fig. 7. Density of States of Carbon nanotube with chirality (3,0)

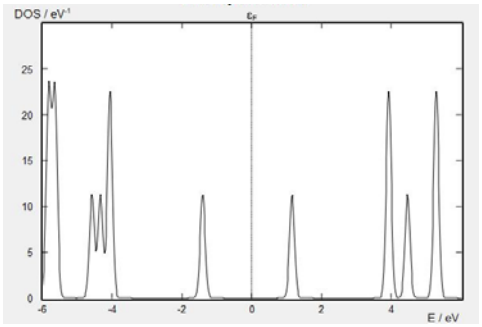

Fig. 8. Density of States of Carbon nanotube with chirality (3,3)

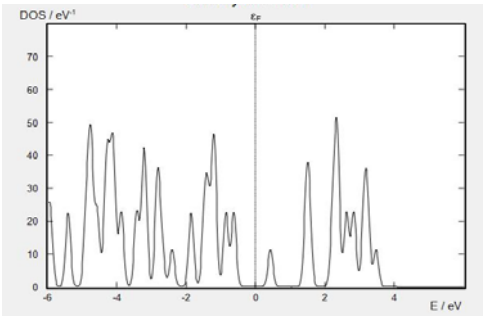

Fig. 9. Density of States of Carbon nanotube with chirality (3,2)

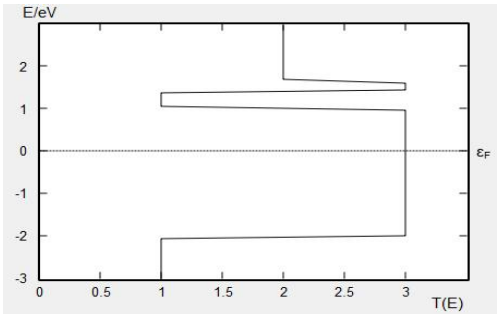

Fig. 10. Transmission spectrum of Carbon nanotube with chirality (3,0)

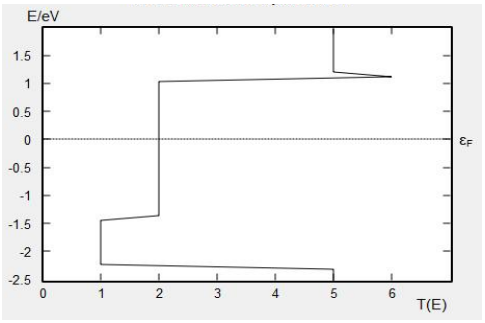

Fig. 11. Transmission spectrum of Carbon nanotube with

chirality (3,3)

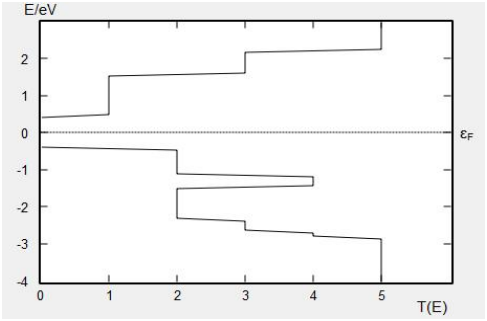

Fig. 12. Transmission spectrum of Carbon nanotube with chirality (3,2)

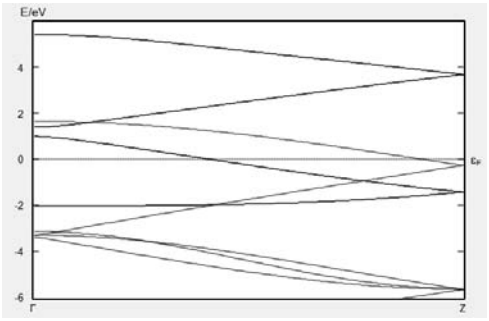

Fig. 13. Band Structure of Carbon nanotube with chirality (3,0)

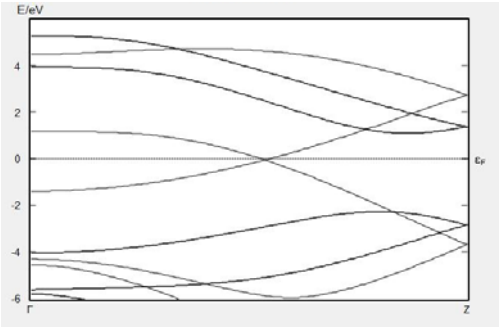

Fig. 14. Band Structure of Carbon nanotube with chirality (3,3)

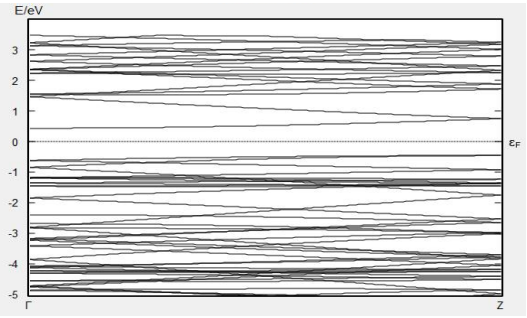

Fig. 15. Band Structure of Carbon nanotube with chirality (3,2)

In Fig. 10, 11, and 12 Transmission spectrum of carbon nanotubes with (3,0), (3,3), (3,2) chirality are shown. From the Transmission spectrum of the carbon nanotube we can determine the energy of bonds when atoms are grown along the nanotube's length. We observed that for carbon nanotube with chirality (3,0) when adding carbon atoms to the nanotube the bond energy between the newly added atom and each of the existing adjacent atoms is equal to one another. The carbon nanotube with chirality (3,0) has better energy transmission spectrum.

In Fig. 13, 14, and 15 the Band Structure of carbon nanotubes with the above mentioned chirality is shown. For nanotubes with chirality (3,2) and (3,0) DFT (Density Functional Theory) with LDA (Local Density Approximation) is used for calculation of the Band Structure. For nanotubes with chirality (3,3) the Hückel calculation method is used. The k-points are set to 5x5x5 for n_a, n_b, n_c, respectively.

IV. Conclusion

We performed analysis of Carbon nanotubes with zig zag (3,0) chirality, armchair (3,3) chirality, and Chiral (3,2) chirality. The analysis showed that tubes with (3,0) chirality have better energy bond, tubes with (3,2) chirality have more energy levels into their Brillouin zone. Transmission spectrum of carbon nanotubes with (3,0) is best among the other chiralities that we have examined.

Acknowledgement

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References

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