Impact of changing channel length and band gaps of a carbon nanotube on the current of a Carbon Nanotube Field Effect Transistors (CNTFETs)

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Abstract:

This paper introduce a new way to simulate the effect of changing the length and the band gap of the nanotube on the current of carbon nanotube field effect transistors (CNTFET) by using simulation tools: FETToy, CNTFET lab, CNT bands 2.0, since this simulation were done in different parameters of ZigZag nanotube. We use three simulations tools because each tool provides simulation of parameters that differ from the parameters of other tools, so we can study more parameters that we change which this article is studied.

In this paper we studied the effect of changing of ZigZag nanotube length which has a chirality (n,0) on the current of the CNTFET. We have found that the relationship between nanotube length and the current of the CNTFET is an inverse proportional, as the nanotube length increase, the current of CNTFET decrease, and the relation between the band gap of the ZigZag nanotube and current of the CNTFET has been studied too. We have found that this relationship is an inverse proportional, as the band gap increase, the current of CNTFET decrease. Also, we studied the relation between the band gap of the ZigZag nanotube and the average velocity of charges in CNTFET, we found that relationship is an inverse proportional, as the band gap increase, the average velocity of charges of CNTFET decrease.

Key Words: Nanotube Length, Band Gap, Average Velocity of Charges, Chirality, CNTFET

دراسة تأثير تغير طول الأنبوب النانوي وفجوة الطاقة على تيار ترانزستورات الأثر الحقلي المصنعة من الأنابيب النانوية (CNTFET)

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الخلاصة:

يقدم البحث طريقة جديدة لمحاكاة تأثير تغير طول الأنبوب النانوي وفجوة الطاقة على تيار ترانزستورات الأثر الحقلي المصنعة من الأنابيب النانوية (CNTFET) وذلك باستخدام أدوات المحاكاة FETToy وCNTFET lab و CNT bands 2.0 حيث ستتم هذه المحاكاة عند بارامترات مختلفة للأنابيب النانوية، حيث أننا قمنا باستخدام ثلاث أدوات للمحاكاة لأن كل أداة منها تمكن من محاكاة بارامترات مختلفة عن الأداة الأخرى وبالتالي نستطيع في هذه الحالة دراسة عدد أكبر من تغير البارامترات التي تهدف هذه المقالة إلى دراستها.

درسنا في هذه المقالة تأثير تغير طول الأنبوب النانوي نوع ZigZag والذي تكون معاملات التوجيه فيه Chirality من الشكل (n,0) على تغير تيار الترانزستور CNTFET، حيث وجدنا أن العلاقة هي علاقة عكسية بين طول الأنبوب النانوي والتيار في الترانزستور CNTFET، فكلما ازداد طول الأنبوب النانوي يتناقص التيار في هذا الترانزستور، وكذلك درسنا العلاقة بين فجوة الطاقة في الأنبوب النانوي نوع ZigZag وتيار الترانزستور CNTFET، حيث وجدنا أن هذه العلاقة هي علاقة عكسية، فكلما ازدادت فجوة الطاقة في الأنبوب النانوي يتناقص التيار في هذا الترانزستور، والعلاقة بين تغير فجوة الطاقة في الأنبوب النانوي نوع ZigZag ومتوسط سرعة الشحنات في الترانزستور CNTFET تمت دراتها أيضا، حيث وجدنا أن العلاقة هي علاقة عكسية بين فجوة الطاقة في الأنبوب النانوي ومتوسط سرعة الشحنات في CNTFET، فكلما ازدادت فجوة الطاقة في الأنبوب النانوي يتناقص متوسط سرعة الشحنات.

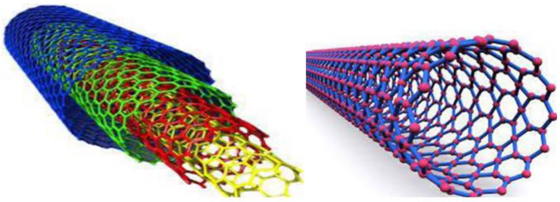
كلمات مفتاحية: طول الأنبوب النانوي، فجوة الطاقة، متوسط سرعة الشحنات، معاملات التوجيه، ترانزستورات CNTFET.

1-Introduction

Carbon nanotube (CNTs) are cylindrical carbon nanostructures discovered by Japanese physicist Sumio Ijima [1]. It has unique structural, mechanical and electronic properties.

The nanotubes are divided into single-walled and multi-walled nanotubes [2]. Single-walled carbon nanotube (SWCNT) was manufactured in 1993 and Multi-walled carbon nanotube (MWCNT) was manufactured in 1991 [3].

SWCNT has a smaller diameter between (0.4-2 nm) and a length up to 1.5cm and can be metallic or semiconductor, whereas the diameter of MWCNT ranges between (10-200 nm) and a length up to hundreds of microns [3] and it is metal. Fig.1 shows single-walled and multi-walled nanotubes [3].



a b

Figure 1 : a) multi-walled nanotube b) single-walled nanotube

2-Single-Walled Carbon Nanotube (SWCNT):

The structure of an ideal (infinitely long) single-walled carbon nanotube is that a regular hexagonal lattice drawn on an infinite cylindrical surface, whose vertices are the positions of the carbon atoms. Since the length of the carbon-carbon bonds is fairly fixed, there are constraints on the diameter of the cylinder and the arrangement of the atoms on it [4]. Its electronic properties change dramatically with the chirality (n, m), which indicate to how the graphene sheet is rolled to form the carbon nanotubes [5].

The diameter of SWCNT is given by the relation [6].

$$d_{(SWNT)}(nm) = 0.0783\sqrt{n^2 + m^2 + nm} \qquad (1)$$

The band gap of the SWCNT can be given by the relation [6]:

$$E_g(eV) = \frac{2\gamma_0 a_{c-c}}{d_{(SWNT)}} = \frac{0.852}{d_{(SWNT)}} \qquad (2)$$

Where $\gamma_0 = 3eV$ (constant) The bonding energy between a carbon atom and a neighboring one, and (a_{c-c} =0.142nm) is the length of the C-C bond and it is constant too.

Single-walled carbon nanotubes can be divided according to the Chirality (n,m) into two types:

1- Chiral (can be metal or semi-conductor).

2- Archiral and includes two types:

Armchair (Metal)

Zigzag (can be metal or semi- conductor)

This division follows the direction of the rolled up the sheet of graphene to form the nanotubes, and hence the value of the Chirality n and m [5]. Fig.2 shows examples of single-walled nanotube types.

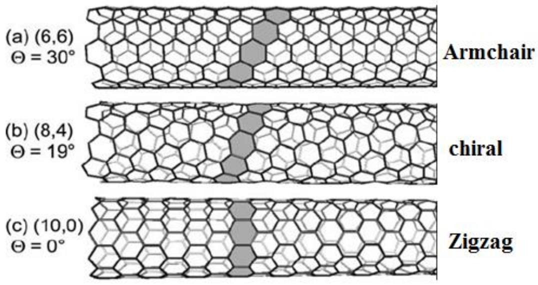


Figure 2: Examples of single-walled carbon nanotube types

Table (1) shows the electrical conductivity of single-walled nanotubes types due to Chirality (n, m).

Table 1: Electrical conductivity of nanotubes

Electrical conductivity	Nonotube	Chirality (n, m)
It is metallic when n is multiple of 3, Otherwise it is semiconductor		)n,0(
Always metalic		)n,n(
It is metallic when $\frac{2n+m}{3}$ is an integer number, otherwise it is semiconductor		(n,m) where m≠0

3- Multi-Walled Carbon Nanotube (MWCNT):

Multi-walled carbon nanotubes (MWCNTs) consist of multiple layers of graphene. Its structure is complex and has great structural diversity compared to SWCNTs. However, MWCNTs have advantages over SWCNTs, such as ease of mass production, low product cost per unit, and enhanced thermal and chemical stability [7]. MWCNT structural stability plays a crucial role in nanodevices and nanotechnology. The hollow, cylindrical, and distinctive flawless curved graphitic carbon nanotube (CNT) structure with sp^2 hybridized atomic bonding makes them exceptional in mechanical strength, electronic properties, and a potential material candidate for nanodevices and other areas of nanotechnology [8].

In general, the electrical and mechanical properties of SWNTs can change when functionalized, due to the structural defects occurred by C=C bond breakages during chemical processes. However, intrinsic properties of carbon nanotubes can be preserved by the surface modification of MWNTs, where the outer wall of MWNTs is exposed to chemical modifiers [7].

4-Double-Walled Carbon Nanotubes:

There is another type of carbon nanotube, it is called Double-Walled Carbon Nanotube. It is blend of both single-walled and multi-walled nanotubes, showing properties intermediate between the two types. DWNTs are comprised of exactly two concentric nanotubes separated by 0.35 – 0.40 nm, with sufficient band gaps for use in field-effect transistors [9]. The inner and outer walls of DWNTs have optical and Raman scattering characteristics of each wall [10].

Theoretically, if each wall behaves like a SWNT, DWNTs can consist of four combinations based on the electronic type (metallic or semiconducting) according to (n, m) values of their inner and outer walls, e.g., metallic-metallic (inner-outer), metallic-semiconducting, semiconducting-metallic, and semiconducting-semiconducting. Some experimental studies found that even though both walls are semiconducting, DWNTs may behave as a metal [11].

This complication of their overall electrical behavior has limited the utility of DWNTs to applications such as thin film electronics. However, DWNTs also exhibit several beneficial properties observed from MWNTs, such as improved lifetimes and current densities for field emission and high stability under aggressive chemical, mechanical, and thermal treatments along with the flexibility observed with SWNTs [12].

5- Simulation Results:

The chirality (n, m) in the nanotube plays a major role in changing the properties of the nanotube used in field effect transistors (CNTFETs) and therefore greatly affect the different parameters of these transistors, the energy gap, the number of atoms, the number of bonds, and also affect the diameter of the nanotube, which affects the current of the CNTFET transistor, the velocity of charges, the conductivity, threshold voltage and all parameters of the CNTFET transistor.

When considering the effect of changing the chirality (n, m) on the performance of the CNTFET transistor, the length of the nanotubes is constant, but the length of the nanotubes is one of the most important parameters that must to pay attention to when designing CNTFET transistors, as it represents the channel length in this transistor. We have studied the effect of changing the length of the ZigZag nanotubes on the drain current in the CNTFET transistors, and examined the effect of the energy gap change in the nanotube on the drain current and the average charge speed of this transistor, using the FETToy, CNTFET lab and CNT bands 2.0 simulation tools.

5-1- Studying the effect of changing the length of the Zigzag nanotube on the drain current of the typical CNTFET transistor:

Using the CNTFET Lab simulation tool we examined the effect of the length of the nanotube on the drain current in the typical CNTFET transistor as shown in Figure 3:

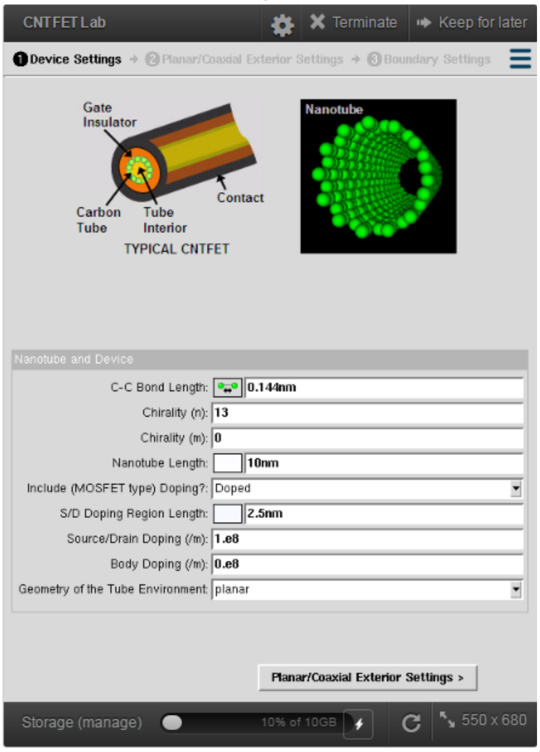


Figure 3: typical CNTFET transistor in CNTFET Lab simulation tool

The following basic parameters are introduced:

- The length of the C-C bond is 0.144nm.
- Chirality (n, m) = (13,0) so it is a ZigZag nanotube.
- At first we introduced the length of the nanotube equal to 10nm.

And we have maintained the other parameters as it is in this simulation tool which are shown in Fig.4.

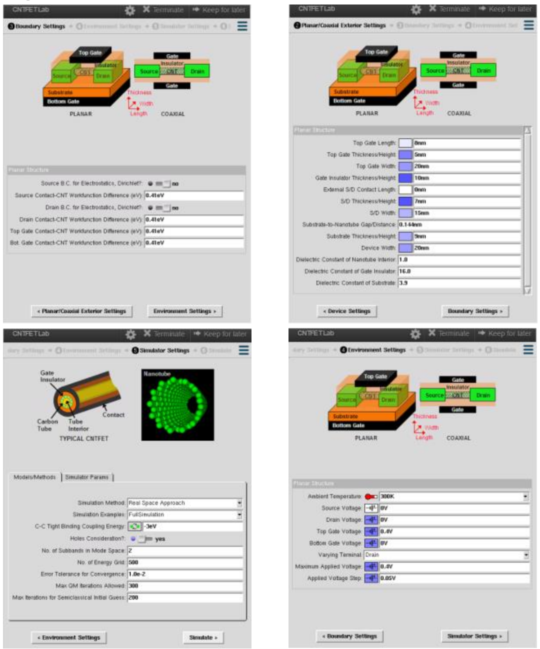


Figure 4: parameters of simulation

Figure 5 shows the relationship between V_{GS} and the drain current at the length of the ZigZag (13,0) nanotubes equal to 10nm.

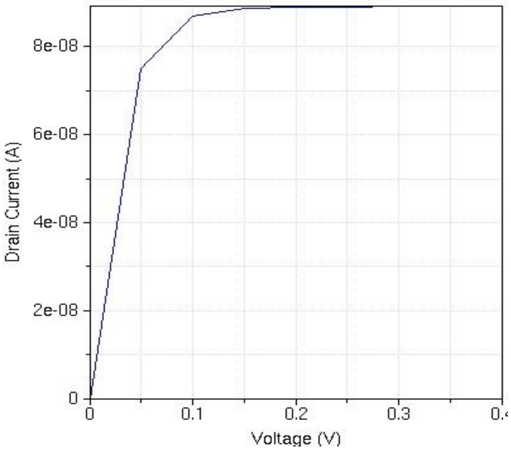


Figure 5: I_d=f(V_{GS}) at the length of the (13,0) nanotubes equal to 10nm.

By changing the length of the nanotube to the following values: 5nm, 20nm and 50nm, we get Figs. 6-8.

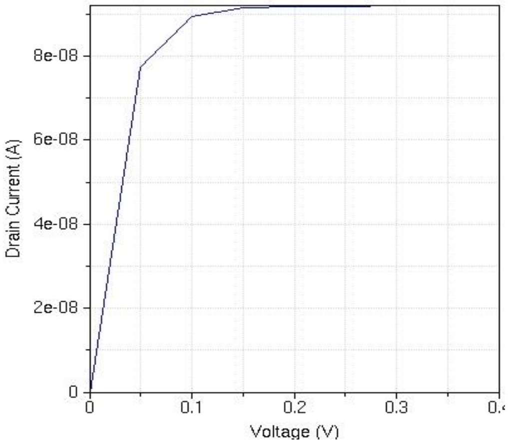


Figure 6: I_d=f(V_{GS}) at the length of the (13,0) nanotubes equal to 5nm.

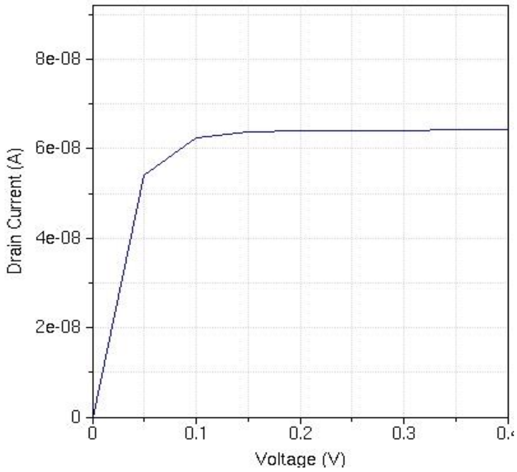


Figure 7: I_d=f(V_{GS}) at the length of the (13,0) nanotubes equal to 20nm.

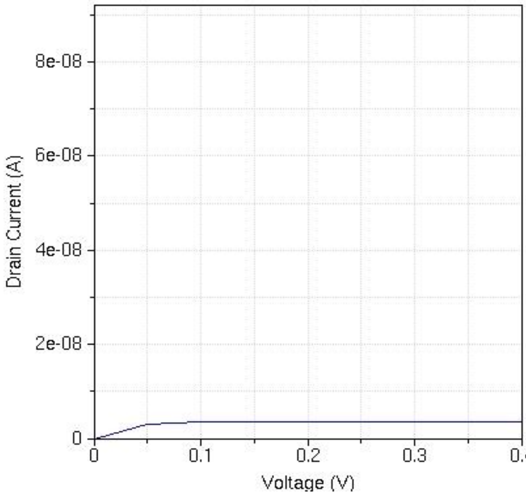


Figure 8: I_d=f(V_{GS}) at the length of the (13,0) nanotubes equal to 50nm.

We summaries these results in table 2 where we consider the current values at V_{GS}=0.4V that means the values when the current reach the saturation.

Table 2: I_d values due to various nanotube (13,0) length

L (nm)	50	20	10	5
Id $\times 10^{-8}$	0,4	6,3	8,9	9,2

Using Graph software, we plot the relationship between the length of the nanotube and the drain current in the CNTFET transistor, which is shown in Fig.9.

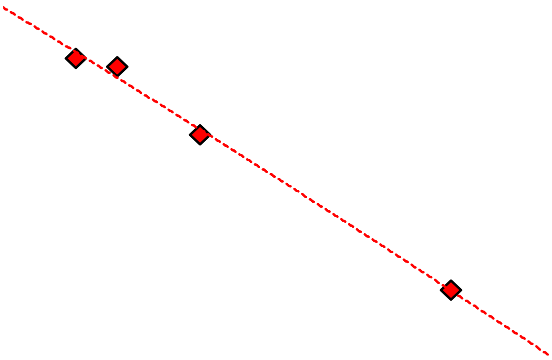


Figure 9: The relationship between the length of the nanotube (13,0) and the drain current in the CNTFET transistor

We note that the relationship is inverse proportional, the longer the length of the nanotube, the less current of the drain in the transistor CNTFET, and this relationship is close to the linear relationship somewhat.

By changing the chirality of the nanotube to (5,0), we find Fig. 10 and Fig. 11:

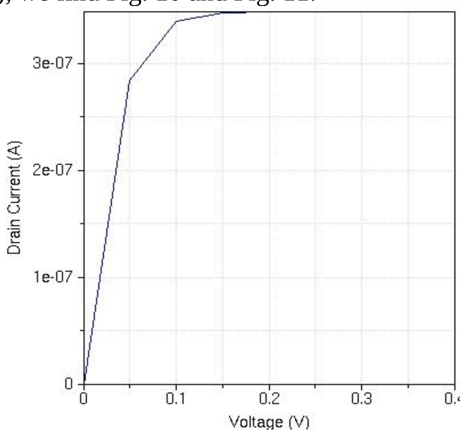


Figure 10: $I_d=f(V_{GS})$ at the length of the (5,0) nanotubes equal to 5nm.

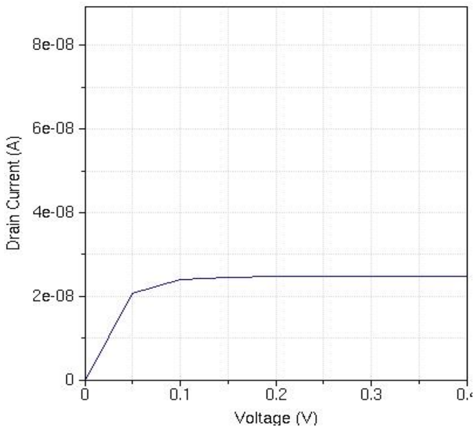


Figure 11: $I_d=f(V_{GS})$ at the length of the (5,0) nanotubes equal to 10nm.

We summaries these results in table 3 where we consider the current values at V_{GS}=0.4V that means the values when the current reach the saturation.

Table 3

Table 3: I_d values due to various nanotube (5,0) length

L (nm)	10	5
Id	2.5×10^{-8}	4×10^{-7}

We note that the drain current in the CNTFET transistor decreases with increasing nanotube length.

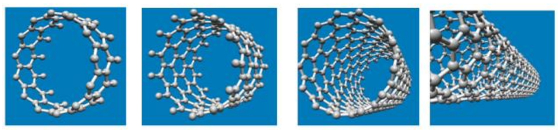
Using the nanotube modeler software, we can enter the chirality of the nanotube, and enter the length of the nanotube and find out the number of atoms and the number of bonds. Also, we can draw the nanotubes, and determine the length of the bond between the carbon atoms, and this software enable us to obtain the diameter of the nanotube, we can find the nanotube diameter for the chirality (13,0) and (5,0) as shown in the table 4.

Table 4: the nanotube diameter for the chirality (13,0) and (5,0)

Chirality (n,0)	(13,0)	(5,0)
Nanotube diameter (nm)	1,0185	0.3917

We find that the nanotubes (13,0) are larger in diameter than the nanotubes (5,0). This relationship to various nanotubes was studied in a previous study [5]. it was proved that the correlation between chirality and the diameter of the nanotubes is direct proportional.

Figure 12 shows the nanotube (13,0) in different length as we obtained from nanotube modeler software.



5nm 10nm 20nm 50nm

Figure 12: various length of nanotube (13,0)

5-2 Studying the effect of changing energy gap of the Zigzag nanotubes on the CNTFET transistor drain current.

First: Using the CNTbands 2.0 simulation tool, We studied the band structure diagram of several types of nanotubes [5]. This diagram shows the energy gap (which represents the difference in energy between the conductivity band and the valence band) in the nanotube. The band gaps of CNTs are small (from 0.2 to 2.0 eV), so CNTs are either metallic or semiconductive [13].

Figure 13 shows the band structure diagram of some nanotubes according to their chirality.

The (5,0) and (10,5) nanotube acts as semi conducting material since it has energy gap between conduction and valence band. The (10, 10) and (10, 4) nanotube act as conducting material as the valance and conduction bands are overlapping. (Table 5).

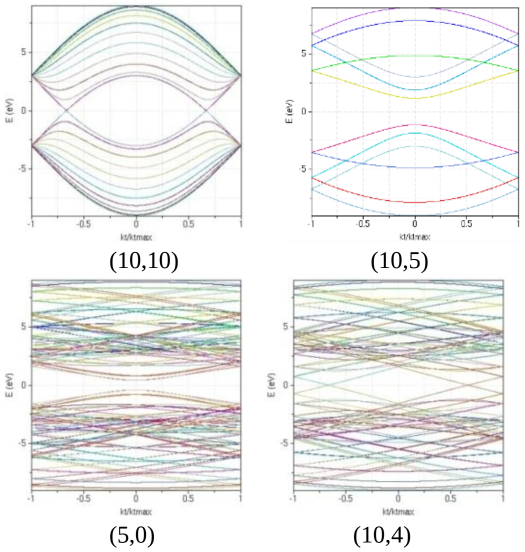


Figure 13: the band structure diagram of some nanotubes according to their chirality.

Using this simulation tool we can obtain the energy gap and the diameter and the chiral angle (which represent the direction of rolling the grapheme sheet to form the nanotube) of the nanotube for various chirality, we summaries these results in table 5.

Table 5: nanotube diameter and energy band and chiral angle due to Nanotube chirality

Nanotube chirality	Nanotube diameter (nm)	Energy Band (eV)	Chiral angel (degree)
(3,3)	0.4068	0.01088	30
(5,5)	0.687	0.010880	30
(7,7)	0.9492	0.01088	30
(6,6)	0.8136	0.010880	30
(10,10)	1.356	0.010880	30
(5,0)	0.39144	2.2918	0
(6,0)	0.46973	0	0
(7,0)	0.54802	1.4849	0
(10,0)	0.78289	1.0534	0
(6,4)	0.68251	1.2543	23.413
(6,5)	0.74683	1.1285	26.996
(10,4)	0.97783	0.0030185	16.102
(10,5)	1.0357	0.83064	19.107
(10,6)	1.096	0.76849	21.787

Using a Graph software we plot the relationship between the energy gap and the diameter of the semiconductor zigzag nanotube which is shown in Figure 14.

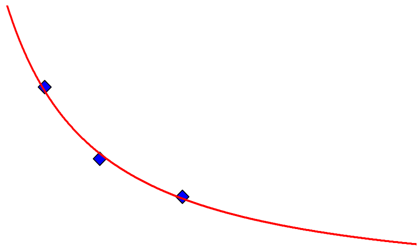


Figure 14: Relationship between the energy gap and the diameter of the semiconductor Zigzag nanotube

From this figure, we find that the energy gap in this semiconductor nanotubes depends on the diameter of the tube and is inversely proportional to it. Where the diameter 0.39144 nm corresponds to a nanotube (5,0), the diameter 0.54802 nm corresponds to a nanotube (7,0) and the diameter 0.78289 nm corresponds to a nanotube (10,0).

Second: Using the FETToy simulation tool, by simulating a CNTFET transistor with a nanotube chirality (5,0), (7,0) and (10,0) we get the relationship between V_{GS} and the drain current as shown in Figures 15 and 16 and 17, where we fixed the V_{DS} value to 1V, and introduced the following simulation parameters:

- •Threshold voltage 0.32V.
- •Gateway Control Parameter 0.8 (AlphaG)
- •Bank Control Parameter 0.035 (AlphaD)
- •Temperature 300K.
- •Gate insulator thickness (tins) 1.5nm.
- • gate insulator dielectric constant 3.9.

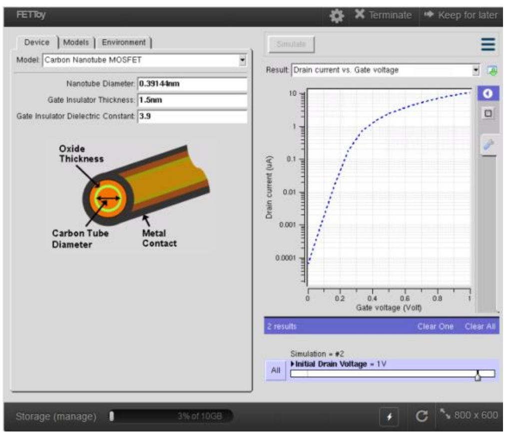


Figure 15: The relation between gate voltage and drain current for CNTFET with (5,0) nanotube

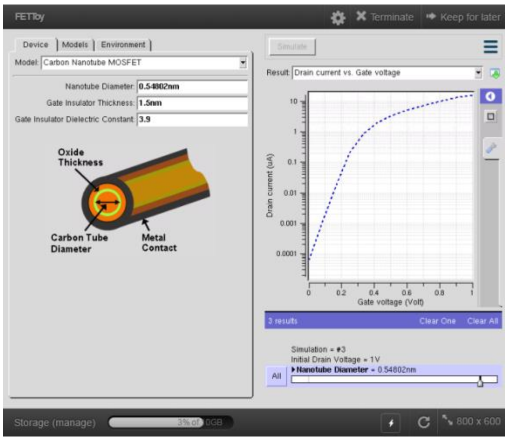


Figure 16: The relation between gate voltage and drain current for CNTFET with (7,0) nanotube

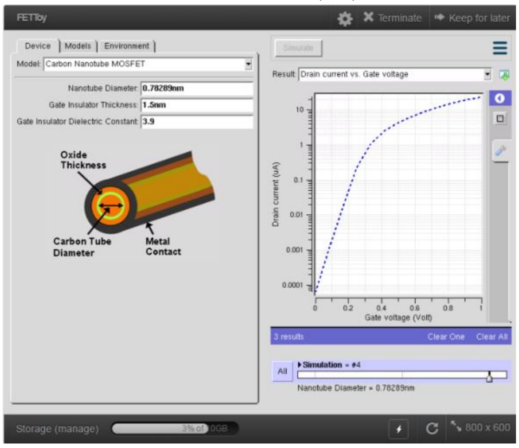


Figure 17: The relation between gate voltage and drain current for CNTFET with (10,0) nanotube

Combining the three images together we find Figure 18, (where we fixed the voltage V_{DS} = 1V).

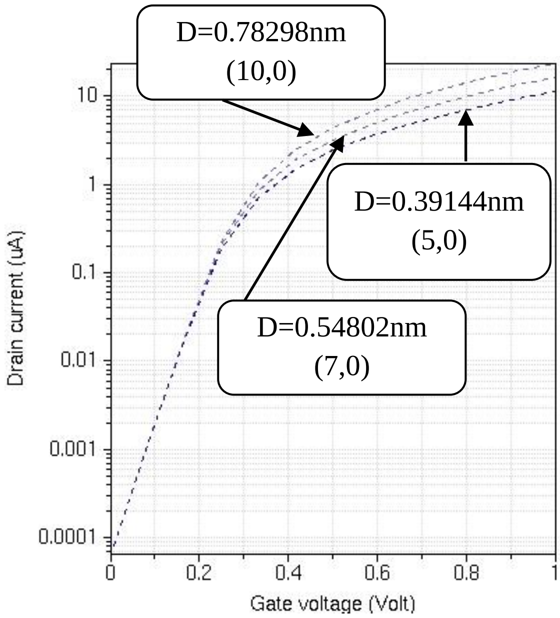


Figure 18: drain current versus gate voltage with different diameter of nanotube

We note that the greater the diameter of the nanotube, the more current in the CNTFET transistor. we summarize the results in Table 6, where the value of the current was at V_{GS} = 0.5V.

Table 6: drain current versus gate voltage with different diameter of nanotube when V_{GS} = 0.5V

D (nm)	0.78298	0.54802	0.39144
Id (µA)	4.37	3.22	2.43

If we choose another value for V_{GS}, for example V_{GS}= 1V, we find the results shown in Table (7):

Table 7: drain current versus gate voltage with different diameter of nanotube when V_{GS} = 1V

D (nm)	0.78298	0.54802	0.39144
Id (µA)	23.9	16.3	11.2

We refer here that the current value when V_{GS} = 1V and V_{DS} = 1V is called the current I (on).

<u>Third</u>: Using the results obtained in table 5 (or figure 15) and Table 7, the above can be summarized in Table 8, which shows the drain current in the CNTFET transistor (at V_{GS} = 1V) with the energy gap in the nanotube at different diameters of the Zigzag nanotube.

Table 8: drain current and energy gap with various diameter of nanotube

Diameter Chirality	Drain current (µA) CNTFET	Energy Gap (eV)
D=0.39144nm (5,0)	11.2	2.2918
D=0.54802nm (7,0)	16.3	1.4849
D=0.78298nm (10,0)	23.9	1.0534

Using Graph software, we plot the relationship between the drain current and the energy gap in the ZigZag nanotube, as shown in figure 19.

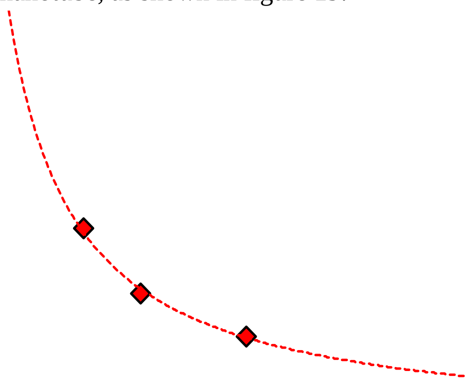


Figure 19: relationship between the drain current and the energy gap in the ZigZag nanotube

We find that the relationship between the energy gap and the current of the CNTFET transistor is inverse proportional, the greater the energy gap, the lower the current of the drain into the CNTFET transistor.

5-3 Studying the effect of changing the energy gap in the ZigZag nanotubes on the average charge velocity in the CNTFET transistor.

Using the FETToy simulation tool we plotted the relationship between V_{GS} and the average charge speed in the CNTFET transistor. At the same parameters in 4-2 (Second) ,so we get Figure 20.

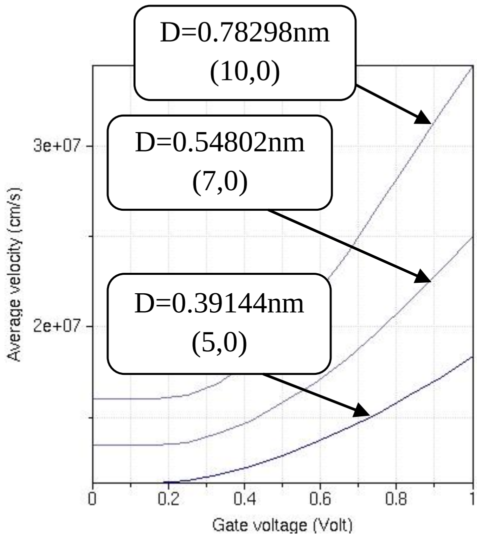


Figure 20: the relation between gate voltage and average velocity in CNTFET with different diameter of nanotube

If we take the average charge velocity at gate voltage = 1V and at V_{DS} = 1V we get the table 9.

Table 9: the average charge velocity with different nanotube diameters

D (nm)	0.78298	0.54802	0.39144
Average charge velocity $\times 10^7$(cm/s)	3.46	2.52	1.87

Using the results obtained in table (5) and table (9), the above can be summarized in Table 10, which shows the average charge velocity in the CNTFET transistor (at V_{GS} = 1V) with the energy gap in the nanotube at different diameters of this Zigzag nanotube.

Table 10: average charge velocity and energy gap with various diameter of nanotube

Diameter Chirality	average charge velocity in CNTFET cm/s	Energy Gap (eV)
D=0.39144nm (5,0)	$1.87.10^7$	2.2918
D=0.54802nm (7,0)	$2.52.10^7$	1.4849
D=0.78298nm (10,0)	$3.46.10^7$	1.0534

Using graph software we plot the relationship between the average velocity of charges in the CNTFET transistor and the energy gap, which is shown in figure 21.

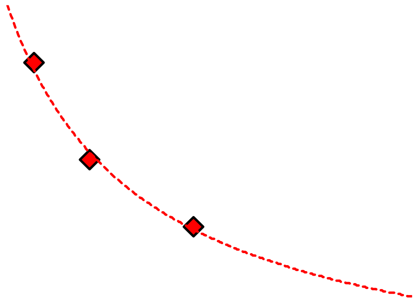


Figure 21: relationship between the average velocity of charges in the CNTFET transistor and the energy gap

From the Fig.21 we note that the relationship between the average velocity of charges in the CNTFET transistor and the energy gap is inverse proportional, that mean the increase in energy gap leading to decrease in average velocity of charges in the CNTFET.

5- Results and discussion:

As a result of our simulation, we found that the relationship between the length of the ZigZag nanotube and the current in the transistor CNTFET is inverse proportional, the more the length of the nanotube decreases the current in this transistor, as well as the relationship between the energy gap in the ZigZag nanotube and the current of the transistor CNTFET, is inverse proportional, as the energy gap in the nanotube increases and the current decreases in this transistor. We also found that the relationship between the change of the energy gap in the ZigZag nanotube and the average charge velocity of the CNTFET transistor, which was inverse proportional, the more the energy gap in the ZigZag nanotube decreases the average velocity of charge.

6- Conclusions

Changing the chirality (n,m) in the nanotube changes the properties of the nanotube used in CNTFETs and therefore greatly affects the performance of these transistors, as well as changing the length of the nanotube significantly affects the performance of CNTFET transistors. Energy gap is an important factor in determining the conductivity of nanotubes and thus affects the performance of CNTFET transistors. Thus, a trade off between different parameters of the CNTFET nanotube should be found depending on the application required.

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