

Characteristic control of SWCNT-FET by varying its chirality and dimensions

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ABSTRACT

Carbon nanotube (CNT) has witnessed great importance due to its electronic and mechanical properties. The CNTFET was designed to provide high-performance electronic devices. Therefore, the carbon nanotube is representing a potential material for future microelectronic devices. In this paper, COMSOL Multiphysics was used to design and a simulate single-walled carbon nanotube field-effect transistor with a back gate. As the CNT was not included in the material library of COMSOL, its electrical parameters were input manually, including relative permittivity, band gap, electron affinity, effective density of states in the valence and conduction band, electron, and hole mobility. The insulation layer used in the model was silicon dioxide. The influence of changing its thickness on the drain current was discussed. In addition, the specification of carbon nanotubes was investigated in terms of changing their diameter and length. Moreover, this paper reveals the current transport of CNTFET for different applied gate voltage and drain voltage. In our work, the CNTFET behaves as n-type FET with transconductance $g_m \approx 1.25 \mu A$ and electron mobility equal to $4.77 \times 10^{-26} \text{ cm}^2 \text{ v}^{-1} \text{ s}^{-1}$. To obtain semiconducting properties for the CNT material, it must consider the chirality when altering the carbon nanotubes diameter. In the proposed device, the diameter values range from 1nm to 4.5nm. It was found that increasing the diameter range resulted in decreasing bandgap from 0.497 eV to 0.110 eV and increasing drain current from 4.075 μA to 31.33 μA

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1. INTRODUCTION

Carbon nanotube field-effect transistors have gained a great importance recently because of their superior electrical, mechanical, and thermal feature [1-8]. The formation of the covalent bonds sp^2 between atoms of carbon results in exceptional mechanical characteristics. Carbon nanotube is a seamless hollow tubes made from rolling graphite sheets that are separated into single-walled and multi-walled carbon nanotubes [9, 10]. The transport in carbon nanotubes is ballistic that is the electron doesn't suffer any scattering of its energy in the form of photons. There are three types of single-wall carbon nanotubes, depending on the method of folding (Zigzag, Armchair, Chiral). The development of single-walled CNTFETs has made significant progress (SWCNTFET) due to their unique properties, where it bows elastically (rather than fracture) under enormous bending or compressive forces. Many technologies are being considered to aid in miniaturizing transistors, carbon nanotubes have the potential to help [11, 12].

The demand for tiny devices with greater operating speeds has arisen because of technological advancements in all sectors of life. The scaling of silicon should be altered, so silicon MOSFET has been gradually replaced by carbon nanotube field-effect transistors (CNTFET). CNTFET is classified based on

geometry into four classifications, which are back gate CNTFET, top gate CNTFET, wrap around gate CNTFET, and suspended CNTFET[13]. D. Yang et al [14], a fabrication process of CNTFET by applying AC Dielectrophoretic (ACDEP) to form the conductive channel by deposit and aligning SWCNT a strong performance was created (on/off ratio= 10^6) it has steady electrochemical characteristics and a dependable I-V profile. K. R. Sonkusare et al [15], Investigated the performance of the CNTFET by simulating its main parameters. The diameter and thickness of the gate insulator were changed. This could lead to a prediction of the performance of a device, which could result in building complex circuits consisting of CNTFETs. It was found that there was a decrease in current-carrying efficiency when nanotube diameter decreased, while there was an improvement in the current-carrying efficiency due to thinning gate insulator. A. Soares et al [16], Design and simulate a quantum carbon nanotube field-effect transistors based on top-gated to get the excellent electrical characteristics for sub 5nm technologies. R. Hegde et al[17], designed a piezoresistive pressure sensor that is made of both single-walled and multi-walled carbon nanotubes polymer nanocomposite to compare their sensitivity. They found the sensitivity of the pressure sensor made of SWCNTs is three times that of MWCNTs, and that the resistance increase linearly with the increasing application for both SWCNTs and MWCNTs.

In this paper, a simple and accurate method was proposed to design and simulate a single-wall carbon nanotube field-effect transistor based on geometrics variation based on COMSOL simulator . The feature of this model is to obtain the I-V characteristics of CNTFETs, and current transport which are affected by changing the diameter, length of CNTs, and the thickness of silicon dioxide. Since the library of COMSOL doesn't have the CNT, we add the CNT as a new material to the library of the COMSOL this is done by adding full properties of CNT including relative permittivity, band gap, electron affinity, effective density of states in the valence and conduction band, electron and hole mobility to the library. We also found that the electron properties of FET transistor can be changes by changing the bandgap of the CNT and we found that the bandgap is inversely proportional of the CNT.

2. MODELING OF A SINGLE WALL CARBON NANOTUBE FIELD-EFFECT TRANSISTOR

The method that used to determine the diameter, bandgap, and the threshold voltage of SWCNT is defined by the chirality vector C_h with (n, m).

$$C_h = na_1 + ma_2 \quad (1)$$

In this case, the lattice basis vectors a_1 and a_2 are combined linearly to form the chiral vector C_h . The chiral indices are vectors with positive integers n and m. Basically, chiral indices are used to calculate the diameter and bandgap of SWCNT[18], The diameter is derived by,

$$d = \frac{\sqrt{3} a}{\pi} \sqrt{n^2 + m^2 + 2nm} \quad (2)$$

Where, $a=0.142\text{nm}$ is the space between adjacent carbon atoms. The bandgap in SWCNT, which depends on its diameter [19] is determined by:

$$E_g = \frac{2aV_{pp\pi}}{\sqrt{3} d} \quad (3)$$

Where, $V_{pp\pi} = 3.033\text{eV}$ is the carbon π - π bond energy[20]. The threshold voltage can be computed as follows[21],

$$V_{th} = \frac{E_g}{2e} = \frac{\sqrt{3}}{3} \frac{e}{2} \frac{V_{pp\pi}}{d_{CNT}} = \frac{0.436}{d_{CNT}} \quad (4)$$

The transport in a carbon nanotube is ballistic, that is, the electron doesn't suffer from any scattering of its energy in the form of phonons. the resistance of ballistic transport is given by the following equation[22]:

$$R_Q = \frac{h}{e^2} = 26 \text{ K}\Omega \quad (5)$$

While the ballistic conductance can be found Landauer formula[23]:

$$G = e^2/h \cdot \sum_{i=1}^M t_i(E_F) \quad (6)$$

Furthermore, the drain current can be derived from Landauer formula [24]

$$I_d = \frac{2Q}{h} \int_{-\infty}^{\infty} (f(\varepsilon - \varepsilon_{FS}) - f(\varepsilon - \varepsilon_{FD})) T(\varepsilon) d\varepsilon \quad (7)$$

Where, h is the plank's constant, f is the fermi-function, ε_{FS} , ε_{FD} is Fermi level in source and drain, the transmission coefficient $T(\varepsilon)$ measures the likelihood of carriers connecting with one other. The electron mobility μ of the CNT can be estimated using the equation [25]

$$\mu = \frac{L_{\text{CNT}}^2 g_m}{C_g V_d} \quad (8)$$

Where, L is the length of CNTs, g_m is the transconductance and C_g is the gate capacitance that can be calculated by:

$$C_g = 2\pi L_{\text{CNT}} \varepsilon_r \varepsilon_0 / \ln(2t/r) \quad (9)$$

Where, ε_r is the dielectric constant of silicon dioxide, t is thickness of silicon dioxide

3. DESIGN AND SIMULATION OF CNTFET

A SWCNT- FET with back gate was designed and simulated using COMSOL Multiphysics. Figure 1 shows the schematic of the back gate of SWCNT-FET. In this work a SWCNT is formed by rolling-up a single layer of graphene (hollow cylindrical). The CNT was connected between two metal electrodes (source and drain). The source and drain were made of gold with a thickness of 50nm. This structure was constructed on a silicon dioxide (300nm) over silicon substrate (2uA). The silicon substrate was doped by Boron to obtain an n-type silicon substrate. The parameters used in our design are shown in table 1.

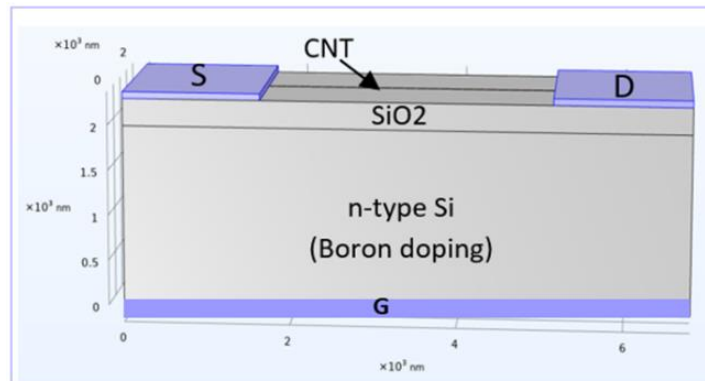
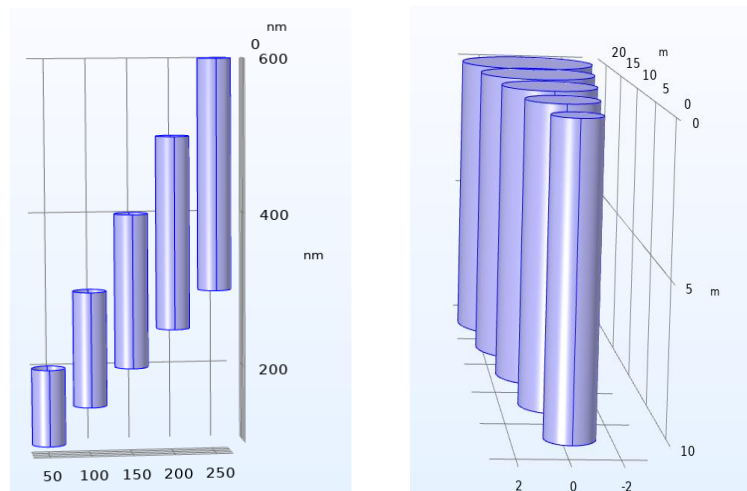


Figure 1. Schematic of CNTFET in COMSOL Multiphysics



(a)

(b)

Figure 2. Schematic diagram of CNT with different (a) lengths (b) diameter

Table 1. The parameters of SWCNT transistor used in COMSOL Multiphysics

Parameters	Value
Thickness of CNT	0.345nm
Bandgap of CNT	0.497eV
Diameter of CNT	1nm
Thickness of Silicon dioxide	300nm
Thickness of gold contact	50nm
Thickness of silicon	2000nm
Length of CNT	3500nm
Width of silicon	6800nm
Hole effective mass	$0.5m_o$
Electron effective mass	$0.5m_o$
Temperature	293.15K
Electron affinity of CNT	4V
Electron mobility of CNT	$25cm^2/V.S$
Relative permittivity of SiO ₂	3.9
Relative permittivity of CNT	11
Effective density of state in the conduction band	$(2*(2*\pi*m_e*eff*k_B*const*T)/h_{const}^2)^{(3/2)}$
Effective density of state in the valence band	$(2*(2*\pi*m_h*k_B*const*T)/h_{const}^2)^{(3/2)}$
Drain contact type	Ideal ohmic
Source contact type	Ideal ohmic

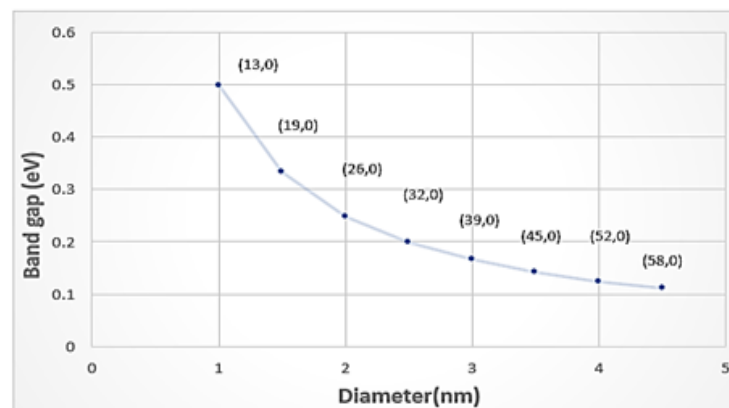
4. RESULTS AND DISCUSSION

The electronic properties of SWCNT are determined by chiral numbers (n, m). Particularly, it can be either metallic or semiconductor, depending on its chirality. The carbon nanotube used for this simulation is a zig-zag nanotube with indices (n,0). The proposed method of finding the diameter depends on the chirality, where each diameter value has an exact chirality value. The bandgap and threshold voltage are inversely proportional to its diameter as shown in table 2.

Table 2. The SWCNT parameters at different chirality

Chirality	Diameter (nm)	Drain current (uA)	Bandgap (eV)	Threshold Voltage (V)
(13,0)	1	4.075	0.497	0.436
(19,0)	1.5	6.604	0.332	0.291
(26,0)	2	9.013	0.248	0.218
(32,0)	2.5	13.168	0.198	0.174
(39,0)	3	17.136	0.166	0.145
(45,0)	3.5	21.487	0.142	0.124
(52,0)	4	26.165	0.124	0.109
(58,0)	4.5	31.33	0.110	0.096

It can be seen from the table 2 that the increasing of the diameter leads to decrease in both bandgap and threshold voltage, while the drain current increased, as shown in figure 3. For example, increasing the carbon nanotube diameter from 1nm to 4.5nm leads to decreasing in the energy bandgap from 0.497eV to 0.110eV which about (five times), this means that one can control the semiconductor properties of CNT by changing the diameter of CNT



(a)

In fact, changing diameter was achieved in our work by rolling a single wall nanotube graphene layer. In this system noticed that the drain current and threshold voltage changes from 4.075uA and 0.436V to 31.33uA and 0.096V, respectively.

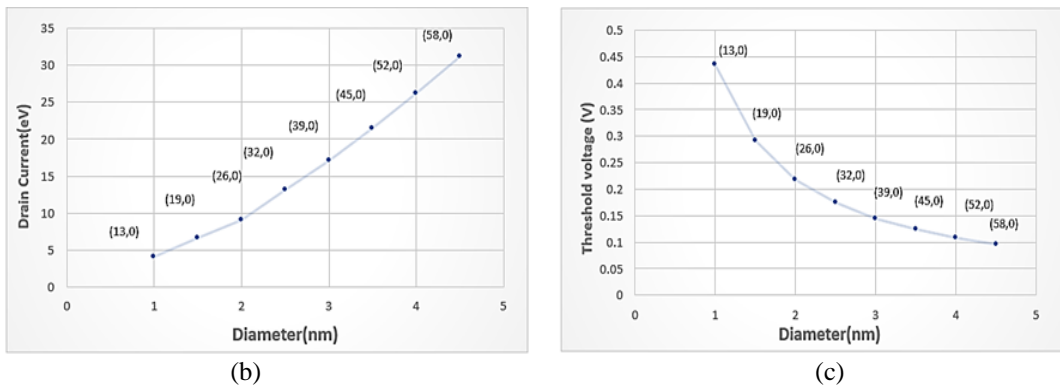


Figure 3. (a) Diameter vs bandgap (b) diameter vs drains current (c) diameter vs Threshold voltage

4.1. Current transport of the designed SWCNT-FET

The Id-Vd characteristics of CNTFET are presented in figure 4 (a,b) for various gate voltage values, and figure 4 (c,d) shows the relationship between (Id-Vg) for different drain voltage values. The influence of changing drain voltage and gate voltage on the drain current was studied.

The CNT parameters that were used to determine the current transport are: diameter is equal to 1nm, the length is equal to 100nm, and the chirality is (13,0). The thickness of the silicon dioxide is equal to 10nm. We observed that the drain current increases with increasing of the drain voltage. Also, when reducing the values of gate voltage, the drain current decreases.

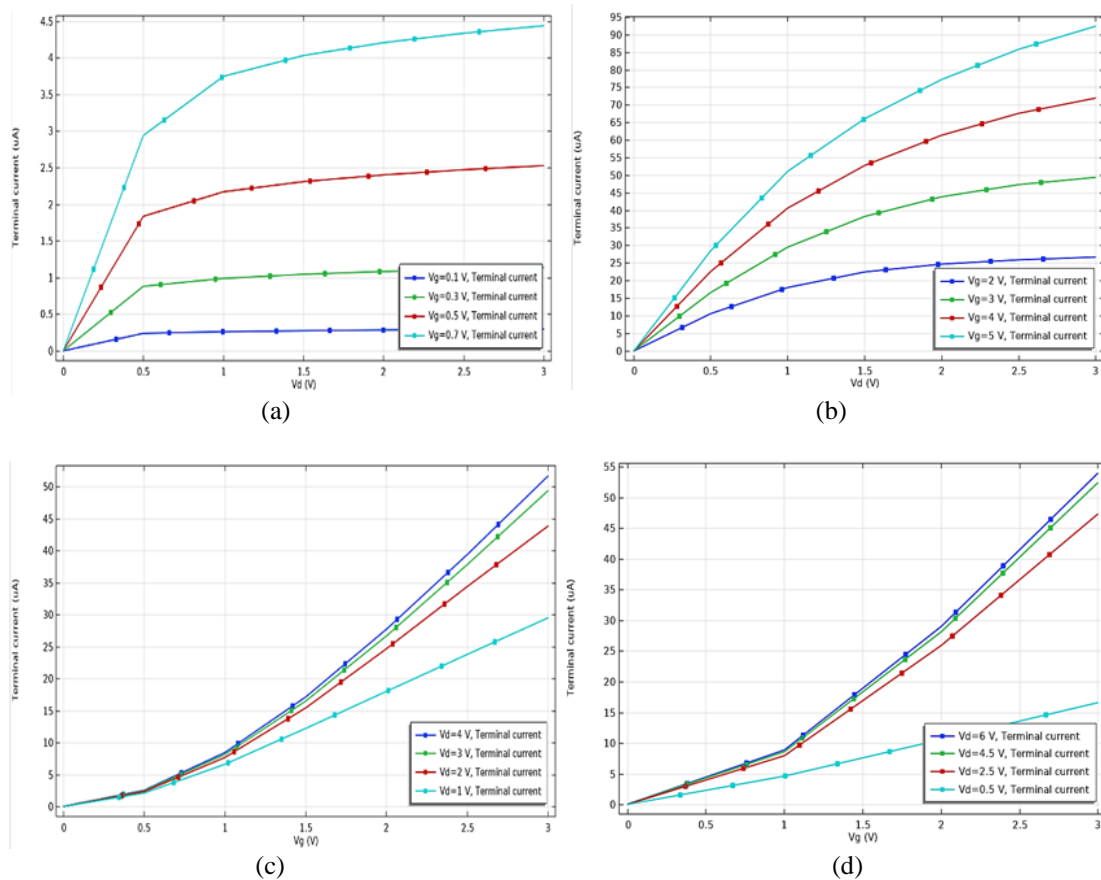


Figure 4. Current transport characteristics (a) Id-Vd at gate voltage (0.1 ,0.3 ,0.5,0.7) (b)Id-Vd at gate voltage (2,3,4,5) (c) Id-Vg at a drain voltage (1,2,3,4) (d) Id-Vg at a drain voltage (0.5,2.5,4.5,6).

4.2. The effect of various diameter of CNT on the SWCNT characteristics

In this section, current voltage relationship was determined for the range of the diameter length, 1nm to 4.5 nm with the length of 3.5 μm . The thickness of the SiO₂ is 300 nm. Figure 5 shows the Id vs Vd at the gate voltage of 1.5 V. The results show that increasing the value of the carbon nanotube diameter leads to elevation in the drain current.

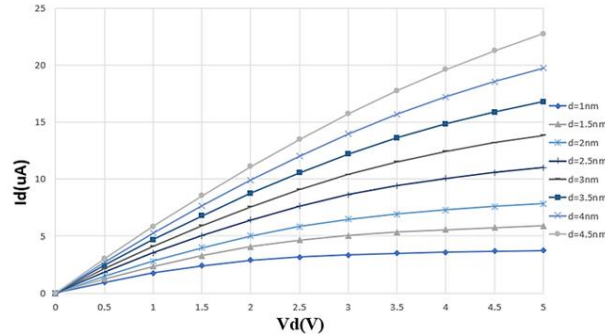


Figure 5. Drain current vs drain voltage at Vg=1.5V

4.3. The effect of various length of CNT on the SWCNT characteristics

To study the effect of changing carbon nanotube length on the drain current, a range of lengths from (32nm to 3500nm) was selected as illustrated in table 3. We found that the drain current increased as the length of CNT decreased. This can be attributed to the decreasing of number of collisions of charge carrier, as explain in equation 8 of the about section. Furthermore, the electron mobility is direct proportional to the length of CNT. The measurement was done at gate voltage of 1.5V. For more investigation of property of CNT, we studied the effect of thickness of silicon dioxide on the current transport of CNT. We figured out that the drain current elevated as the thickness of silicon dioxide get decreased. Figure 6 shows the drain voltage relationship at several CNT lengths.

Table 3. Different lengths of CNT

Length of CNT (nm)	Drain current(uA)
32	1876.996
100	928.38
150	425.77
200	240.29
250	159.30
500	48.94
1000	18.35
1500	11.06
2000	7.8
2500	6.1
3000	4.9
3500	4.1

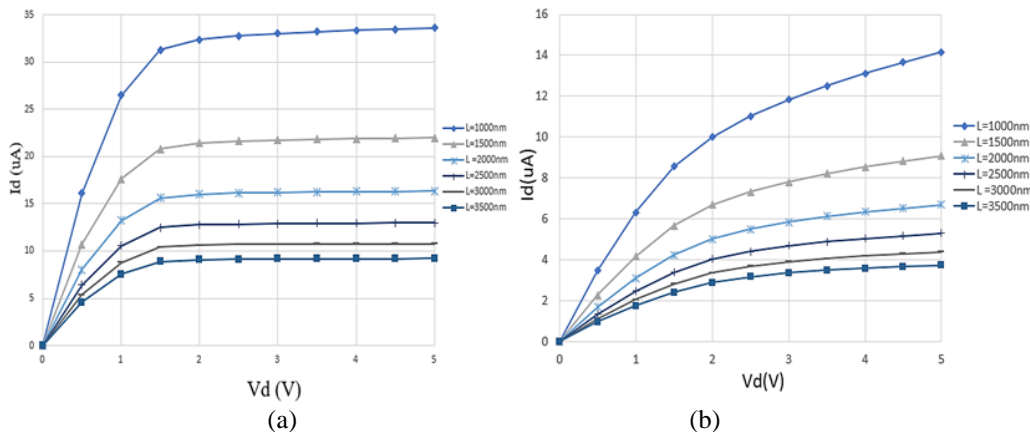


Figure 6. I-V characteristics of different lengths of carbon nanotube (a) oxide thickness is equal 50nm (b) oxide thickness is equal 300nm.

4.4. The effect of various silicon dioxide of CNT on the SWCNT characteristics

In this section, current- voltage characteristics (I_d - V_d) curves were plotted with various values of gate oxide thicknesses, from 1.5nm to 300nm at gate voltage equals to 3V and diameter of CNT of 1nm, as presented in figure 7. The drain current decreases with increasing gate oxide thickness. For example, when the gate oxide thickness increased from 1.5nm to 300nm, the drain current declined to about 53 times.

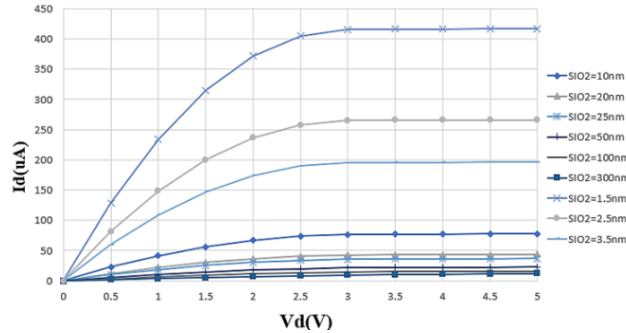


Figure 7. I_d vs V_d at gate oxide thickness from (1.5nm to 300nm)

5. FREQUENCY RESPONSE OF CNTFET

The Performance of carbon nanotube Field -Effect transistors (CNTFETs) was characterized using frequency response to find its bandwidth and the resonance frequency. To estimate the bandwidth of CNTFETs, we utilized f_{-3dB} as a realistic figure of merit. The frequency response of CNFETs influences with parasitic capacitances, at gigahertz frequencies. Cutoff frequency was used to describe the high frequency performance of the transistor. The intrinsic cutoff frequency is determined by $f_c = g_m / 2\pi C_g$. Where, g_m is the transconductance and C_g is the intrinsic gate capacitance. Obviously, the cutoff frequency is directly proportional to the g_m while, it inversely proportional to C_g . Based on our result, the resonance frequency for our designed CNTFET is equal to 50GHz and the bandwidth is equal to 30GHz.

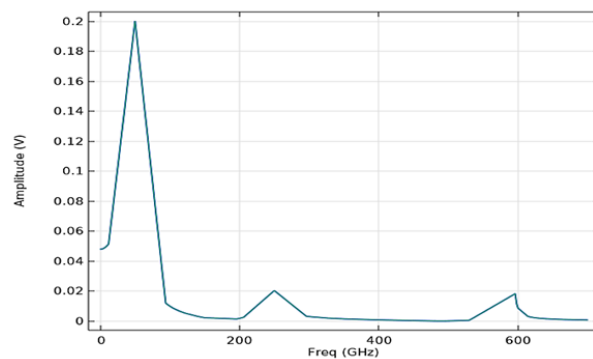


Figure 8. Frequency (GHz) vs Amplitude (V) at Voltage =3V

6. COMPARISON WITH RELATED STUDIES

The obtained results were compared with other previous studies as tabled in table (4).

Table 4. Comparison the results with previous research

Parameter	Our results	FETTOY results [references]	Silvcao TCAD [reference]
Diameter	1nm	1nm [26]	1nm [27]
Gate voltage	1.5V	0.6V [26]	0.8V[27]
Drain current	4.075×10^{-6} A	6.99×10^{-6} [26]	4.75×10^{-3} A [27]
Band gap	0.49eV	- [26]	0.45 eV [27]
Threshold voltage	0.436V	0.245V [26]	0.254V [27]
Transconductance	1.25uA	27uA [26]	- [27]

Table 4. demonstrates that decreasing V_g resulted in massive increase in drain current and transconductance. While the band gap increased slightly with the high increment in the gate voltage. Although equation (4) was adopted to calculate threshold voltage in this research and studies [27] used another equation results were again for the same diameter (1nm).

7. CONCLUSION

This work aims to control the characteristics and specifications of carbon nanotube field effect transistors. In the proposed device, the diameter and length of CNT, as well as silicon dioxide thickness, influence the drain current and bandgap of FET. It was observed that when the diameter is increased, the drain current increases while the drain current is reduced by increasing the length of CNTs. Also, it was noticed that the drain current is equal to (14uA) when the silicon dioxide thickness was 300nm, while it increased to (34uA) when the thickness is equal to 50nm; for the same carbon nanotube length (1000 nm). Additionally, we perceived that the change in diameter is inversely proportional to the bandgap. that altering the bandgap of the CNT may alter the FET transistor's electron characteristics. Furthermore, from the I-V characteristics of CNTFETs, we found that the CNTFETs behave as n-type FET.

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