

# EXPLORING THE ELECTRICAL CONDUCTANCE OF GRAPHENE NANORIBBON AND CARBON NANOTUBES BY VARYING THE BUNDLE WIDTH AND LENGTH TO OPTIMIZE CONDUCTANCE.

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### Abstract

**Aim**: Conductance of graphene nanoribbons and carbon nanotubes are simulated by varying the bundle width from 100 nm to 2000 nm with the step size of 100 nm. **Materials and Methods:** Electrical conductance of Carbon nanotubes (n=100) was compared with graphene nanoribbons (n=100) by varying bundle width of both materials carbon nanotubes and graphene nanoribbons ranging from 100 nm to 2000 nm concerning the length ranging from 2  $\mu$ m to 10  $\mu$ m with the step size of 2  $\mu$ m for each interval of the bundle width in the NANO HUB tool simulation environment. The pre-testing analysis was performed using clinicalc.com with G-power set to 85%, the threshold set to 0.05 for each group, and the sample size set to 100. **Results**: Graphene nanoribbons have significantly higher conductance (120.487 mho, P<0.001) than carbon nanotubes (31.364 mho, P<0.001). The optimal bundle width for the maximum conductivity is 2000 nm for Carbon nanotubes and graphene nanoribbons. **Conclusion:** Within the scope of this study, Graphene nanoribbons with a bundle width of 2000 nm offer the best conductivity.

Keywords: Novel graphene nanoribbons, Carbon nanotubes, Bundle width, Nanomaterial, Nanoelectronics

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## 1. Introduction

The conductance of nanomaterials such as Novel graphene nanoribbons and Carbon nanotubes are being explored through simulation by varying the bundle width and length of the device. Carbon nanotubes and novel graphene nanoribbons are vital for improving the bulk polymer's mechanical, thermal, current, and voltage characteristics. (Todri-Sanial, Dijon, and Maffucci 2016). There are many applications for graphene nanoribbons some of the examples are Liquid crystals, Schottky diodes, Transparent conductive electrodes, Solar cell systems, Light emitting diodes, Field effect transistors, etc. (Katsnelson 2020). Examples for the application of Carbon nanotubes are carbon nanotubes based air, water filtration, thermal conductivity, energy storage, carbon nanotubes based MOSFETs, carbon nanotube biomedical applications, etc (Amin, Kumar, and Belharouak 2020).

In the past five years, several articles published in the field of nanoelectronics such as Carbon nanotubes 64 journal papers published in the IEEE explore and 1980 research articles were published in science direct and google scholar. Graphene nanoribbons feature low electrical resistivity, excellent thermal conductivity, and high current and voltage carrying capabilities, making graphene a viable alternative for replacing conventional materials in the fabrication of VLSI nanointerconnects. (Todri-Sanial, Dijon, and Maffucci 2016; Tiwari and Shukla 2014).Graphene nanoribbons are of potential use in the development of electronic and optoelectronic devices (Song and Zeng 2015). GNR shows a bandgap that can be tuned by tailoring its width and edge structure. Zigzag GNRs are always metallic, while armchair GNRs can be either metallic or semiconducting (Kausar 2021). Carbon nanotubes and novel graphene nanoribbons have both demonstrated excellent results in terms of thermal management, RC delay, and conductance at one or more interconnect levels. (Soldano, Talapatra, and Kar 2013).

Our institution is passionate about high quality evidence based research and has excelled in various domains (Vickram et al. 2022; Bharathiraja et al. 2022; Kale et al. 2022; Sumathy et al. 2022; Thanigaivel et al. 2022; Ram et al. 2022; Jothi et al. 2022; Anupong et al. 2022; Yaashikaa, Keerthana Devi, and Senthil Kumar 2022; Palanisamy et al. 2022).Downsizing elements to less than 100 nm in size, as well as connectivity, present numerous significant obstacles. As the interconnect, dimensions approach the lateral dimension, grain boundary scattering, surface scattering, and a high resistivity diffusive barrier layer increase the total resistivity. This study aims to determine the best carbon allotropy such as carbon nanotubes or graphene nanoribbons for interconnecting applications and replace the conventional copper interconnect with it.

## 2. Material and Methods

This study was carried out at the Saveetha University, nano hub simulation lab, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Chennai. In this research, there are two groups in this study. Group 1 refers to carbon nanotubes, whereas Group 2 refers to novel graphene nanoribbons. The pretesting analysis was performed using clinicalc.com with G-power set to 85%, the threshold set to 0.05 for each group, and the sample size set to 100. The overall sample size for the study project is 200, with an 80 percent pre-test power analysis. (Todri-Sanial, Dijon, and Maffucci 2016).

To prepare the sample for group 1, the bundle width is varied from 100 nm to 2000 nm using the nano hub tool at 100 nm step size, in order to analyze the electrical conductance of carbon nanotubes. To simulate the carbon nanotube conductance first open the Nano Hub in any one of the available search engines. Select the resources in the Nano hub home page then select the carbon in tags and select carbon nanotube interconnect in the next box and click on launch in the next box. After launching the tool select the carbon nanotube interconnects from the drop-down box, then go to the structure and vary the bundle width. For each change on the bundle width with an interval of 100 nm, select on simulating to get results for the respective values.

To prepare the sample for group 2, the bundle width is varied from 100 nm to 2000 nm using the nano hub tool at 100 nm step size, in order to analyze the electrical conductance of graphene nanoribbons. Similar to the sample preparation of group one, select the graphene nano to interconnect from the drop-down box, then go to the structure to vary the bundle width. For each change on the bundle width with an interval of 100 nm, select simulating to get the results based on the respective values.

Nano hub consists of standard commercial nanoelectronics software packages which are simulation tools based on research as well as tutorials, and courses. Nano Hub is an open-source simulation tool. It produces precise, accurate findings since it is a software tool (Klimeck et al. 2011). Carbon nanotubes and graphene nanoribbons are analyzed for their current-voltage characteristics. Keep the height as the constant ( h = 100 nm ) and note down the conductance from the plot obtained during simulation, concerning the

length. Do the same procedure for both the carbon nanotube and graphene nanoribbons. The conductance of the carbon nanotubes and novel graphene nanoribbons are obtained.

#### Statical analysis

Origin and SPSS were the statistical tools used in this study. Plotting graphs for input values and comparing variables is done using Origin while determining the mean, standard deviation, and significant difference is done using SPSS (Landau 2017). In this study, the bundle width and length are independent variables because they are inputs and remain constant even after the other parameters are changed, but the conductance is a dependent variable since it depends on the inputs and varies with each change in the input. This study's analysis is based on an independent T-Test that compares the conductivity of carbon nanotubes and graphene nanoribbons.

#### 3. Results

Current-voltage characteristics of nanomaterials such as carbon nanotubes and graphene nanoribbons for the bundle width (50 nm to 1000 nm) are shown in Fig. 1 and Fig. 2 respectively. For every change in the bundle width of the device, conductance is tabulated by keeping the height of the bundle constant 100 nm. Table 1 and Table 2 refer to carbon nanotubes. In which Table 1 ranges from 100 nm to 1200 nm, Table 2 ranges from 1300 nm to 2000 nm. Table 3 and Table 4 refer to graphene nanoribbons, In which Table 3 ranges from 100 nm to 800 nm, Table 4 ranges from 900 nm to 2000 nm. Fig. 1 and Fig. 2 represent the conductivity of the carbon nanotubes and novel graphene nanoribbons respectively. Fig. 3 represents the comparison graph of conductance of carbon nanotubes and novel graphene nanoribbons. Fig. 4 represents the bar chart comparing the mean (+/- 1SD) conductance of carbon nanotubes and graphene nanoribbons. From Table 1 and Table 2 the conductivity of carbon nanotubes was maximum when bundle width is 2000 nm and bundle length is 2 µm which is 31.3647 mho. From Table 3 and Table 4 the conductivity of the graphene nanoribbons was maximum when the bundle width is 2000 nm and bundle length is 2  $\mu$ m which is 120.487 mho.

Conductivity of the nanomaterial such as carbon nanotubes and graphene nanoribbons was increasing with the increase in the bundle width and decreases with the decrease in the bundle length because there is an increase in the number of free electrons on the surface with greater bundle width, resulting in improved electrical conductivity. From Fig. 3 graphene nanoribbons are more conductible than carbon nanoribbons at the same bundle width.

There is a statistically significant difference between the conductance of the nanomaterial such as carbon nanotubes and graphene nanoribbons since the value of p is less than 0.001 (p<0.001) from table 6. From table 5 the average conductance of the carbon nanotubes is 10.399022 is less than the average conductance of the Novel graphene nanoribbons of 14.577580, which indicates that graphene has better conductivity than carbon nanotubes.

#### 4. Discussion

The conductivity of novel graphene nanoribbons and carbon nanotubes is explored by altering the device's bundle width. The electrical conductance characteristics have been simulated for different bundle widths of the device ranging from 100 nm to 2000 nm with a step size of 100 nm. After evaluating the simulation curves, it was found that an increase in the bundle width causes increases in the conductance for both carbon nanotubes and graphene nanoribbons, and graphene nanoribbons (120.487 mhos) has better electrical conductivity than the carbon nanotubes (31.364 mhos) for the maximum 2000 nm of bundle width.

Hassen Dakhlaoui and Shaffa Almansour have the conductivity of graphene researched nanoribbons with multiple barriers when a voltage is supplied. The researcher concluded that the Electronic conductance of graphene nanoribbons is sensitive to the number of carbon atoms and external voltage and current in them, which allows us to tailor the electronic properties of the graphene-based devices (Wong et al., n.d.). The current conductance of graphene nanoribbons strongly depends on the structure of the graphene (zigzag and armchair) conductance of zigzag and armchair structured graphene nanoribbons V = 1.0eV and V = 0, eV respectively with a constant length of 14nm. Graphene nanoribbons can be either semiconducting or metallic, it depends on the shape. As a result, GNRs can be implemented as both a functional element and a connector in nanodevices, since it has better current and voltage properties (Gorjizadeh, Farajian, and Kawazoe 2009). The growing interest in graphene nanointerconnects drives the search for more precise and efficient models that can account for all quantum effects. such as quantum conductance, quantum capacitance, etc arising at the nanoscale (Lopes, Santos, and Bueno 2021). Giovanni Miano and Antonio Maffucci have researched the current and voltage properties of graphene for interconnect applications (Maffucci, Miano, and Villone 2008)

in the field of nanoelectronics. In nanotechnology, where a few hundreds or thousands of atoms are involved, It is crucial to analyze the nature of interfaces and any potential dynamics that happen at an interface. (Todri-Sanial, Dijon, and Maffucci 2016; Soldano, Talapatra, and Kar 2013).

Factors affecting nanomaterials such as graphene nanoribbons are Novel GNRs that have two open edges at both sides in their structure; this boundary structure makes GNRs more vulnerable to defects than carbon nanotubes. Every GNRs contains local defects or extended disorders, whereas graphene sheets commonly contain few defects (Soldano, Talapatra, and Kar 2013). The limitations to this study are the width of a graphene nanoribbon and a carbon nanotube cannot be increased over 1000 nm (Gorjizadeh, Farajian, and Kawazoe 2009).

Copper, which is currently employed as an interconnecting material, is affected by two major issues: One is due to its inability to handle high current density, while the other is due to higher electrical resistance caused by surface dispersion of electronics, as well as issues caused by grain boundaries. In the future, the problems with copper interconnect can be overcome by replacing the copper interconnect with graphene interconnect for better conductivity and thermal performance.

#### 5. Conclusion

Graphene nanoribbons have significantly higher conductance (120.487 mho, p<0.001) than carbon nanotubes (31.3647 mhos, p<0.001). Conductivity increases with increasing width in graphene nanoribbons and carbon nanotubes, so the bundle width should be maximum for optimal conductance.

#### Declarations

**Conflict of Interest** 

No conflict of interest in this manuscript.

#### **Author Contribution**

Author KP was involved in data collection, data analysis, and manuscript writing. Author DA was involved in the conceptualization, guidance, and critical review of the manuscript.

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## Tables and figure

Table 1. Conductivity of carbon nanotubes by varying the width ranging from 100 nm to 1200 nm, In which the highest conductivity is 18.9 mho at 1200 nm width and 2 µm length.

Exploring the Electrical Conductance of Graphene Nanoribbon and Carbon Nanotubes by Varying the Bundle Width and Length to Optimize Conductance.

wid th (nm )	Leng th (µm)	Conducta nce (mho)	Wid th (nm )	leng th (µm )	conductance( mho)	Wid th (nm )	Leng th (µm)	Conductance( mho)	Wid th (nm )	Leng th (µm)	Conducta nce (mho)
	2	1.51765		2	3.12		2	4.17157		2	6.23922
	4	1.23062		4	2.5299		4	3.8286		4	5.055922
100	6 0.871644 200 6	6	1.7919	300	6	2.7117	400	6	3.58343		
	8	0.654209		8	1.3449		8	2.03532		8	2.58952
	10	0.523367		10	1.0759		10	1.62825		10	2.15162
	2	7.84158		2	9.35922		2	10.9608		2	12.5631
	4	6.35852		4	7.58915	700	4	8.88782	800	4	10.171
500	6	4.50372	600	6	5.37536		6	6.29521		6	7.2155
	8	3.38025		8	4.17078		8	4.72847		8	5.41556
	10	2.7042		10	3.22756		10	3.77987		10	4.33245
	2	14.0808		2	15.6824		2	17.2		2	18.8024
	4	11.4177		4	12.7164		4	13.947		4	15.2463
900	6	8.08715	100 0	6	9.00699	110 0	6	9.87863	120 0	6	10.7989
	8	6.06977		8	6.76015		8	7.14436		8	8.10509
10	10	4.85582		10	5.4081		10	5.93149		10	6.46407

Table 2. C	onductivity o	of carbo	n nano	tubes by varying	the wi	dth rang	ging from 1300 n	m to 20	000 nm,	In which
	the h	ighest o	conduc	tivity is 31.3 mb	o at 200	00 nm w	vidth and 2 µm le	ngth.		

wid th (nm )	Leng th (µm)	Conducta nce (mho)	Wid th (nm )	leng th (µm )	conductance( mho)	Wid th (nm )	Leng th (µm)	Conductance( mho)	Wid th (nm )	Leng th (µm)	Conducta nce (mho)
130	2	20.4039	140	2	21.9216	150	2	23.5239	160	2	25.1255

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0	4	16.545	0	4	17.7756	0	4	19.0749	0	4	20.37336
	6	11.7188		6	12.5940		6	13.057		6	14.4306
	8	8.79547		8	9.44968		8	10.1404		8	10.8308
	10	7.043683		10	7.5594		10	8.11232		10	8.66463
	2	26.6432		2	28.2455		2	29.7632		2	31.3647
	4	21.6042		4	22.9035		4	34.1342		4	25.4328
170 0	6	15.3022	180 0	6	16.2225	190 0	6	17.0941	200 0	6	18.014
	8	11.485		8	12.1757		8	12.8299		8	13.5203
	10	9.188		10	9.74057		10	10.2639		10	10.8162

Table 3. Conductivity of graphene nanoribbons by varying the width ranging from 100 nm to 800 nm, In which the highest conductivity is 6.8 mho at 800 nm width and 2 µm length.

wid th (nm )	Leng th (µm)	Conducta nce (mho)	Wid th (nm )	leng th (µA )	conductance( mho)	Wid th (nm )	Leng th (µm)	Conductance( mho)	Wid th (nm )	Leng th (µm)	Conducta nce (mho)
	2	0.048177 8		2	0.152025		2	0.16122		2	0.811162
	4	0.024088 6		4	0.076012		4	0.180610		4	0.40558
100	6	0.012043	200	6	0.050675	300	6	0.120407	400	6	0.21443
	8	0.011024		8	0.038006		8	0.090305		8	0.20364
	10	0.011024		10	0.015298		10	0.072244		10	0.01365
	2	1.579344		2	2.77094		2	4.49186		2	6.84844
500	4 0.789672	600	4	1.385468	700	4	2.24592	800	4	3.42422	
500 -	6	0.59462	000	6	0.923646	700	6	1.497286	000	6	2.2828
	8	0.394836		8	0.554188		8	1.122964		8	1.7122

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	10	0.315868		10	0.554188		10	0.926475		10	1.365484	
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Table 4. Conductivity of graphene nanoribbons by varying the width ranging from 900 nm to 2000 nm, In which
the highest conductivity is 120.5 mho at 2000 nm width and 2 $\mu$ m length.

<b></b>	1		gnest e	onduct	iuctivity is 120.5 mno at 2000 nm						
wid th (nm )	Leng th (µm)	Conducta nce (mho)	Wid th (nm )	leng th (µm )	conductance( mho)	Wid th (nm )	Leng th (µm)	Conductance( mho)	Wid th (nm )	Leng th (µm)	Conducta nce (mho)
	2	9.2876		2	13.0968		2	17.86408		2	23.7116
	4	4.64938		4	6.5484		4	8.93204		4	11.85578
900	6	3.09958	100 0	6	4.3656	$\begin{array}{c} 110\\ 0\end{array}$	6	5.9547	120 0	6	7.90386
	8 3.0	3.00259		8	3.2742		8	4.46602		8	5.92788
	10	2.3619		10	2.61936		10	3.57282		10	4.74232
	2	30.7548		2	39.15743		2	48.9534		2	60.37383
	4	15.3772		4	19.5675	150 0	4	24.4766		4	30.1818
130 0	6	8.96234	140 0	6	13.0448		6	16.3177	160 0	6	20.0606
	8	7.6888		8	9.7834		8	11.658		8	16.9645
	10	6.154094		10	6.9624		10	9.65478		10	11.3256
	2	70.7884		2	85.378		2	101.9106		2	120.487
	4	35.1589		4	42.689		4	50.9554		4	60.326
170 0	6	23.5962	180 0	6	28.4594	190 0	6	33.9702	200 0	6	40.1625
	8	17.6908		8	21.5698		8	25.4776		8	30.1212
	10	14.15766		10	17.0756		10	20.3822		10	24.0974

Table 5. Comparison of Drain conductance of carbo	on nanotubes and novel graphene nanoribbons. Carbon
nanotubes have mean conductance of 10.399022. Grap	hene nanoribbons have mean conductance of 14.577580.

hanotubes have mean conductance of 10.577022. Graphene hanotubes have mean conductance of 14.577500.											
	Group	Ν	Mean	std.Deviation	std.Error mean						
conductance	Carbon nanotubes	100	10.399022	7.34437461	0.7344376						
	Graphene nanoribbons	100	14.577580	21.8920676	2.1892068						

Table 6. T-test comparison of conductance of carbon nanotubes and novel graphene nanoribbons. Since p < 0.001, there is a considerable difference between the two groups (Independent sample T-Test).

Leven's	Test for E	Equality of <sup>•</sup>		Significa	ance	T-test Equality means	for of	95% confidence interval of Difference			
conduc tance		F	Sig	t	df	One- sided p	Two- sided p	Mean Differe nce	Std. Error Differe nce	lower	upper
	Equal varian ces assum ed	30.419	<0.001	- 1.8 10	198	0.036	0.072	- 4.1785 583	2.3091 178	- 8.7321 789	0.3750 623
	Equal varian ces not assum ed			- 1.8 10	121.00 6	0.036	0.073	- 4.1785 583	2.3091 178	- 8.7500 638	0.3929 472

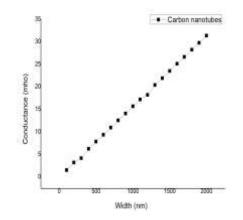


Fig. 1. Simulation of conductance of carbon nanotubes with widths ranging from 50 nm to 2000 nm. The black line represents the conductance of carbon nanotubes.

*Exploring the Electrical Conductance of Graphene Nanoribbon and Carbon Nanotubes by Varying the Bundle Width and Length to Optimize Conductance.* 

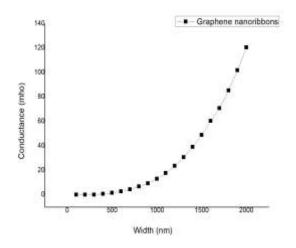


Fig. 2. Simulation of conductance of novel graphene nanoribbons with widths ranging from 50 nm to 2000 nm. The black line represents the conductance of graphene nanoribbons.

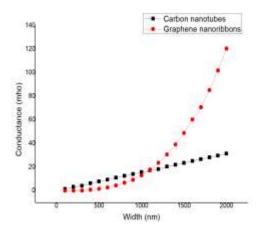


Fig. 3. comparison graph of conductance of carbon nanotubes and novel graphene nanoribbons. The Black line represents the carbon nanotubes and the Red line represents the graphene nanoribbons.

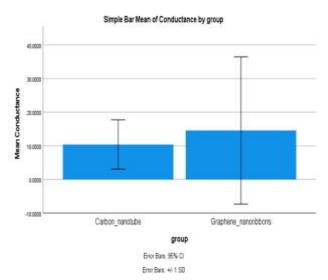


Fig. 4. Bar chart comparing the mean (+/- 1SD) conductance of carbon nanotubes and graphene nanoribbons. The mean conductance of novel graphene nanoribbons is better than carbon nanotubes. X-Axis: carbon nanotubes vs graphene nanoribbons. Y-Axis: Mean of conductance.