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STUDY OF YOUNG'S MODULUS OF GRAPHENE AND ITS DERIVATIVES BY ELASTIC CONSTANTS

[1]**Amit Kumar Yadav**, [2]**Piyush Masih**, [3]**Sarita Khandka**
[1]Research Scholar, [2]Assistant Professor, [3]Associate Professor
[1]Department of Physics,
[1]Sam Higginbottom University of Agriculture, Technology and Sciences, Naini, Prayagraj-211007, Uttar Pradesh, India

ABSTRACT-Young's modulus of graphene and its derivatives is estimated for loadings when force is applied along the armchair direction and when it is applied along the zigzag direction. For young's modulus, elastic constants are used which depends on sample length, width and thickness. So Young's modulus-length graphs are plotted in both the loading cases for graphene and its derivatives. It is found that young's modulus increases with length at constant width and Young's modulus of single layer is greater than double layer. In the case of twisted double layer graphene, Young's modulus decreases with twisting angle.

KEY WORDS - Elastic constant, Young's modulus, twisted graphene & SWNT.

INTRODUCTION - Graphene sheet is a two dimensional plate of carbon atoms organized in a honeycomb structure. It is tightly bound in a hexagonal honeycomb lattice.

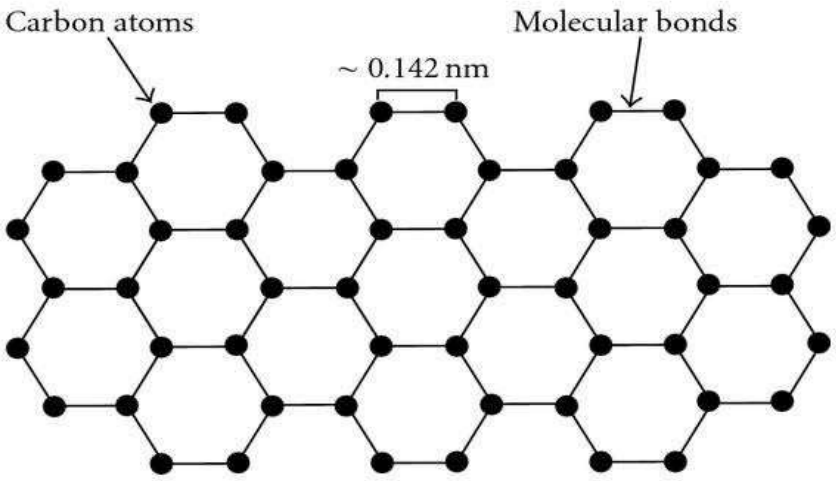

Fig. 1 Schematic structure of a graphene sheet.

In general, the hexagonal structures have five independent elastic constants. These are as follows; C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. C_{11} and C_{12} are more responsible for elasticity. So,

Bulk modulus, $K = \frac{C_{11}+2C_{12}}{3}$ (1.1)

Young's modulus, $Y = \frac{C_{11}^2-C_{12}^2}{C_{11}}$ (1.2)

Now, we can relate the elastic constant and force constant with each other.

Elastic constant, $C_{ij} = \frac{LS_{ij}}{Wt}$ (1.3)

where, A=Wt ,W=width, L=length,t=thickness.
C_{ij} =elastic constant, S_{ij} =force constant.

Hence, Young's modulus, $Y = \frac{(S_{11}^2-S_{12}^2)L}{S_{11}\,Wt}$ (1.4)

Where, S_{11}=133.8391 N/M , S_{12}=8.6127 N/M are force constant for armchair direction. S_{11}=161.481N/M, S_{12}=14.041 N/M are force constant for zigzag direction. Hence, we can calculate young's modulus for different length, width and thickness in different direction.

METHODOLOGY-To analyse the Young's modulus of graphene and its derivatives. We need elastic constants for different length, width and thickness. We have choosen various lengths and widths as well as thickness of different samples. To analyze the effect of shape and size of graphene and its derivatives on Young's modulus, two cases have been taken. Hence,pictorial representation is shown in figure as follow.

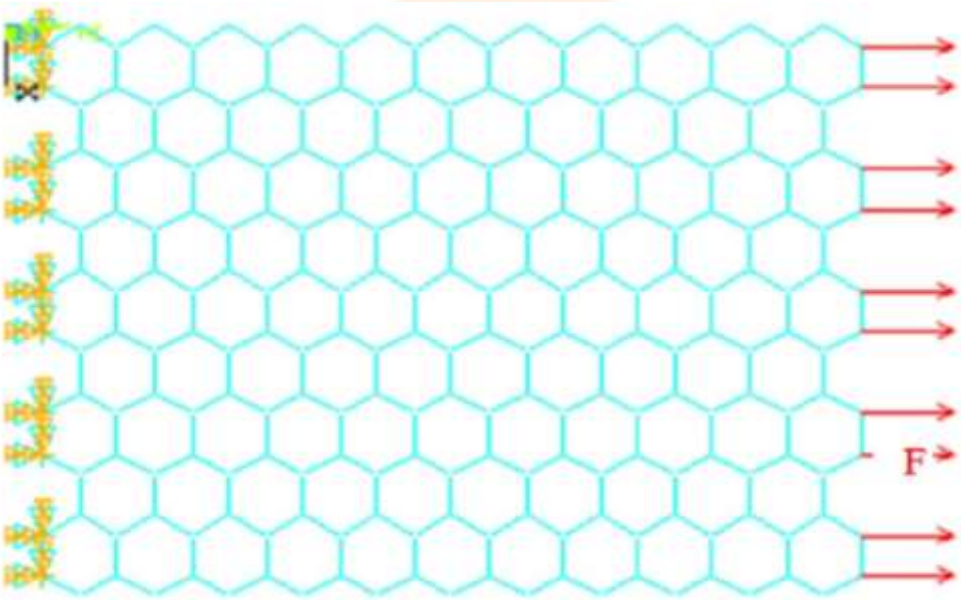

Fig. 2.1 Pictorial representation of loading in which load applied along the armchair direction.

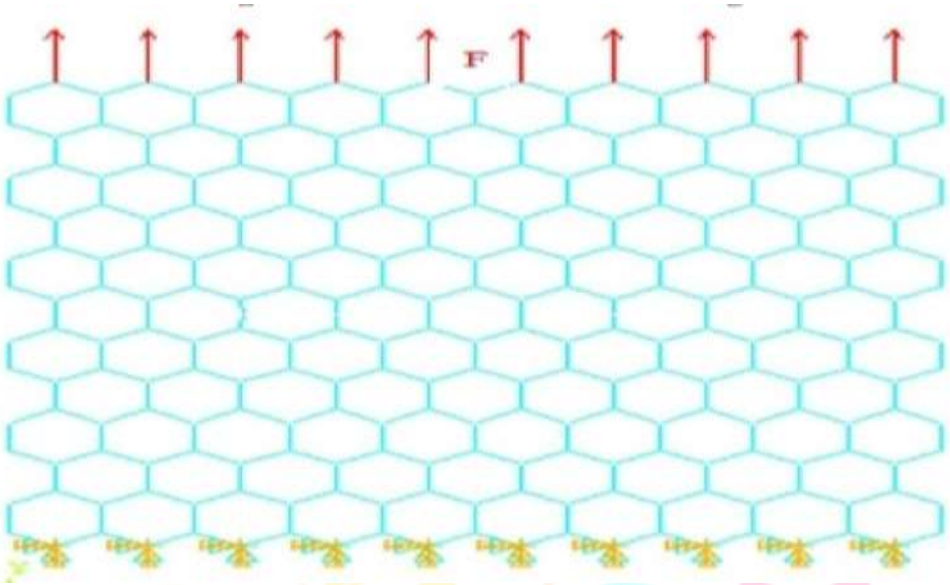

Fig. 2.2 Pictorial representation of loading in which load applied along the zigzag direction.

Now, We have to consider graphene for two cases of loading. 1.47Å thickness of graphene sheet is used.

TABLE 1.1 - Young's modulus for different size of graphene

S.N.	Loading direction	Width(Å)	Length(Å)	$C_{11}(N/M^2)$	$C_{12}(N/M^2)$	Y(TPa)
1	Armchair direction	19.894	56.608	2.5907	0.1667	2.5799
2			118.139	5.4066	0.3479	5.3843
3			177.209	8.1101	0.5218	8.0765
4			238.740	10.9262	0.7031	10.8809
5			297.810	13.6296	0.8770	13.5731
6		41.209	56.608	1.2506	0.0804	1.2455
7			118.139	2.6101	0.1679	2.5993
8			177.209	3.9152	0.2519	3.8990
9			238.740	5.2672	0.3389	5.2454
10			297.810	6.5798	0.4234	6.5525
11	Zigzag direction	24.612	53.998	2.4101	0.2095	2.3919
12			113.680	5.0739	0.4411	5.0356
13			173.362	7.7378	0.6728	7.6793
14			233.044	10.4016	0.9044	10.3230
15			292.726	13.0655	1.1360	12.9667

Now, we have to consider armchair and zigzag direction values for same length.

TABLE 1.1(a)-Comparison of armchair and zigzag direction values						
S.N.	Loading direction	Width(Å)	Length(Å)	$C_{11}(N/M^2)$	$C_{12}(N/M^2)$	Y(TPa)
1	Armchair direction	22.140	51.158	2.1036	0.1353	2.0949
2			110.840	4.5580	0.2933	4.5391
3			170.522	7.0123	0.4512	6.9833
4			230.204	9.4667	0.6091	9.4275
5			289.886	11.9210	0.7671	11.8716
6	Zigzag direction	22.140	51.158	2.5381	0.2206	2.5190
7			110.840	5.4993	0.4781	5.4579
8			170..522	8.4606	0.7356	8.3967
9			230.204	11.4218	0.9931	11.3355
10			289.886	14.3831	1.2506	14.2743

Again, We have to consider double layer graphene for two cases of loading. 3.4Å thickness of double layer graphene is used.

TABLE 1.2 - Young's modulus for different size of double layer graphene						
S.N.	Loading direction	Width(Å)	Length(Å)	$C_{11}(N/M^2)$	$C_{12}(N/M^2)$	Y(TPa)
1	Armchair direction	19.894	56.608	1.1200	0.0720	1.1154
2			118.139	2.3374	0.1504	2.3279
3			177.209	3.5064	0.2256	3.4919
4			238.740	4.7238	0.3039	4.7044
5			297.810	5.8926	0.3791	5.8683
6		41.209	56.608	0.5407	0.0347	0.5385
7			118.139	1.1283	0.0726	1.1238
8			177.209	1.6926	0.1089	1.6856
9			238.740	2.2804	0.1467	2.2710
10			297.810	2.8447	0.1830	2.8330
11	Zigzag direction	24.612	53.998	1.0418	0.0905	1.0341
12			113.680	2.1935	0.1907	2.1771
13			173.362	3.3454	0.2908	3.3201
14			233.044	4.4970	0.3910	4.4631
15			292.726	5.6487	0.4911	5.6061

If we have to consider twisted double layer graphene in which number of ring is equal to ten in armchair direction. When laod is applied along zigzag direction.

TABLE 1.2(a) - Young's modulus for double layer twisted graphene

S.N.	Width(Å)	Θ(Degree)	Y(TPa)
1	24.60	0°	1.0341
2	29.10	7.5°	0.9250
3	33.60	15°	0.8158
4	38.10	22.5°	0.7067
5	42.60	30°	0.5974

If we have to consider SWNT for two cases of loading. 17.054Å,38.369Å and 22.140Å circumference of tube are used.

TABLE 1.3 - Young's modulus for different size of SWNT

S.N.	Loading direction	Cross-section area(Å^2)	Length(Å)	C_{11}(N/M^2)	C_{12}(N/M^2)	Y(TPa)
1	Armchair direction	25.069	54.120	2.8903	0.1859	2.8784
2			115.620	6.1726	0.3972	6.1471
3			174.660	9.3247	0.6000	9.2861
4			236.160	12.6080	0.8113	12.5559
5			295.200	15.7600	1.0141	15.6949
6		56.402	54.120	1.2841	0.0826	1.2789
7			115.620	2.7435	0.1765	2.7322
8			174.660	4.1444	0.2667	4.1273
9			236.160	5.6038	0.3606	5.5807
10			295.200	7.0048	0.4507	6.9758
11	Zigzag direction	32.545	51.158	2.5381	0.2206	2.5190
12			110.840	5.4993	0.4781	5.4579
13			170.522	8.4606	0.7356	8.3967
14			230.204	11.4218	0.9931	11.3355
15			289.886	14.3831	1.2506	14.2743

RESULT DISCUSSION - In the present work, Young's modulus of single layer graphene sheet and its derivatives is calculated using equation (1.2) and equation (1.3) for different width and length of the sheet. The graph is plotted in fig. 3.1,fig. 3.2,fig. 3.3,fig 3.4,fig 3.5 and fig. 3.6 between young's modulus verses length for graphene and its derivatives. It is found from figure that as length increases keeping width constant young's modulus increases. The fig. 3.4(a), fig. 3.4(b) and fig. 3.4(c) show curve for twisted double layer graphene. It is found from figure that as twisting angle increases keeping width constant young's modulus decreases. The fig. 3.2(a) show curve between young's modulus verses length for loading in armchair and zigzag direction, It is found from figure that young's modulus along the zigzag direction is larger than armchair direction. Which is as follow:

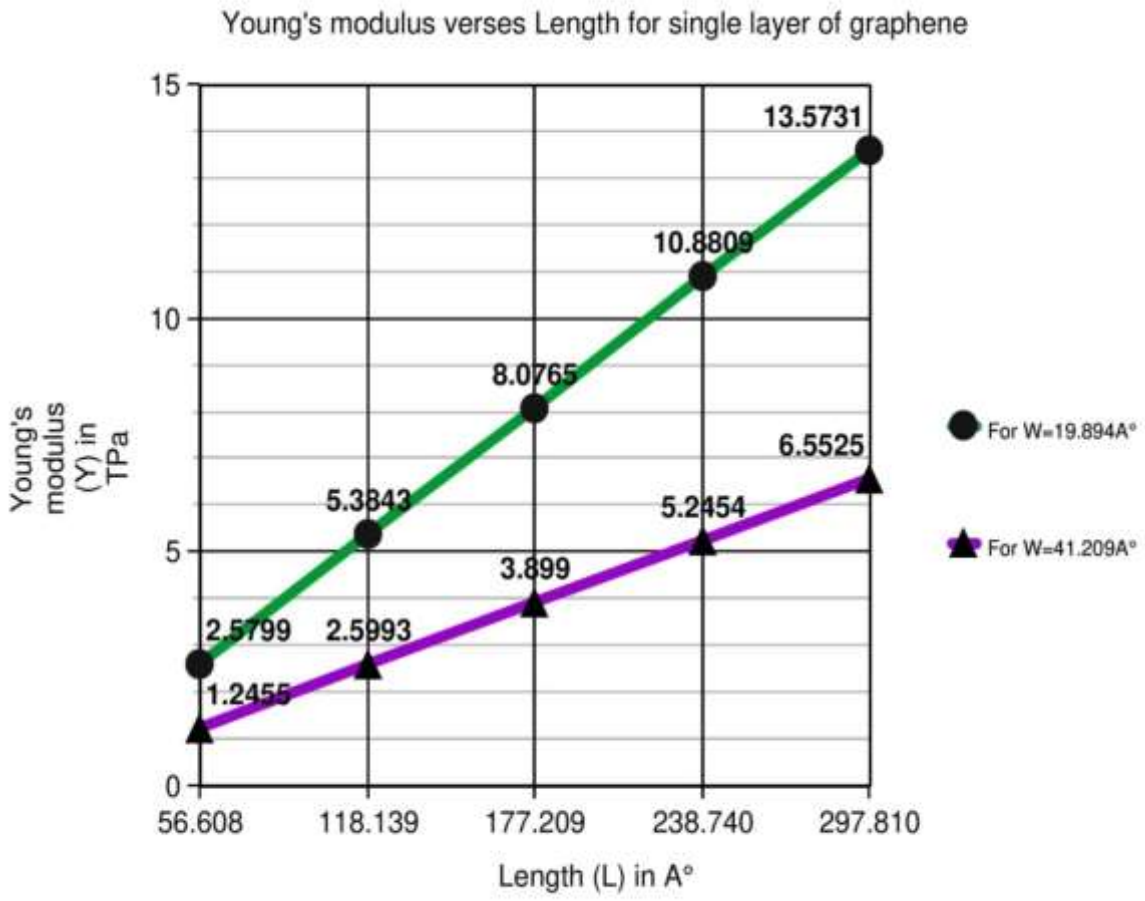

Fig. 3.1 Loading in armchair direction for single layer of graphene

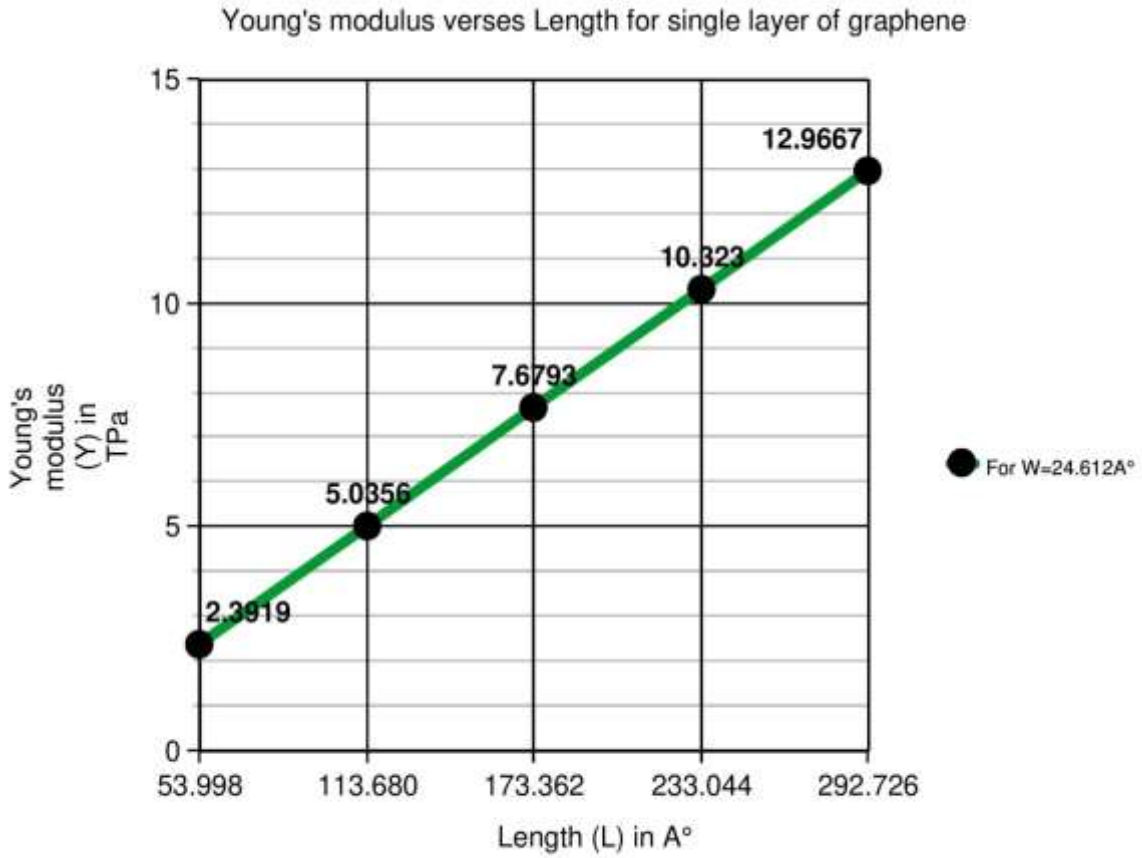

Fig. 3.2 Loading in zigzag direction for single layer of graphene

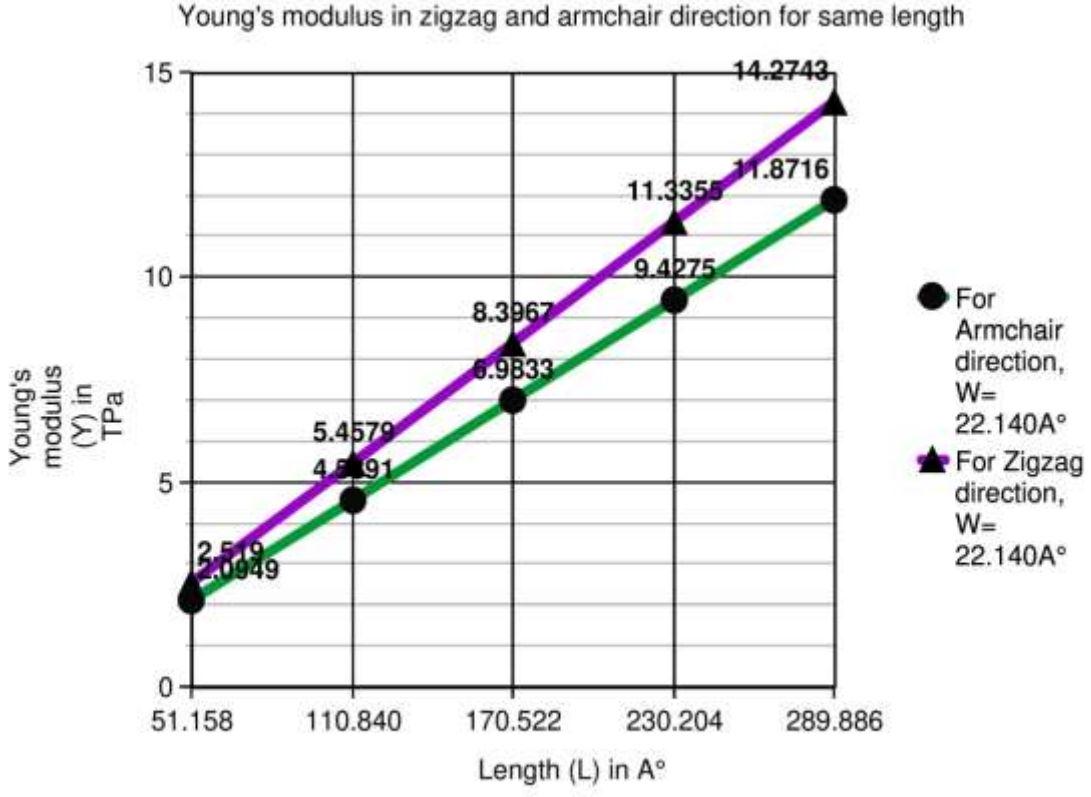

Fig. 3.2(a) Young's modulus in zigzag and armchair direction for same length

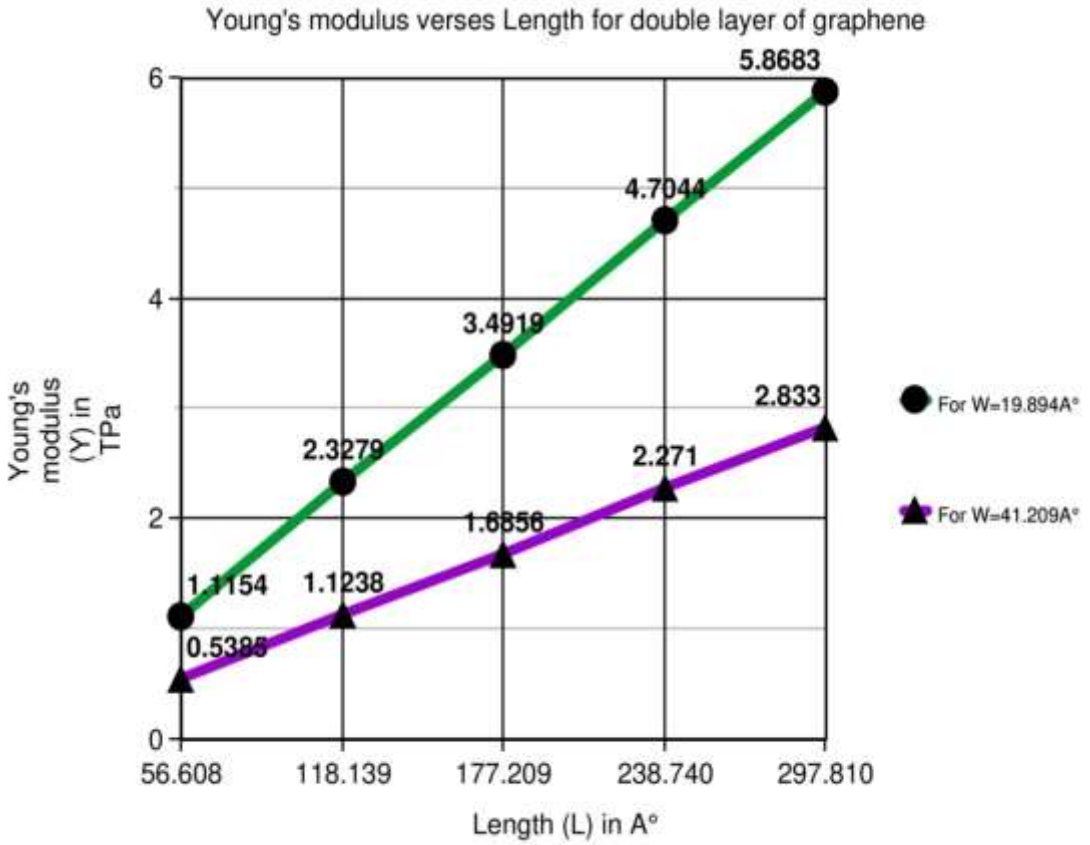

Fig. 3.3 Loading in armchair direction for double layer of graphene

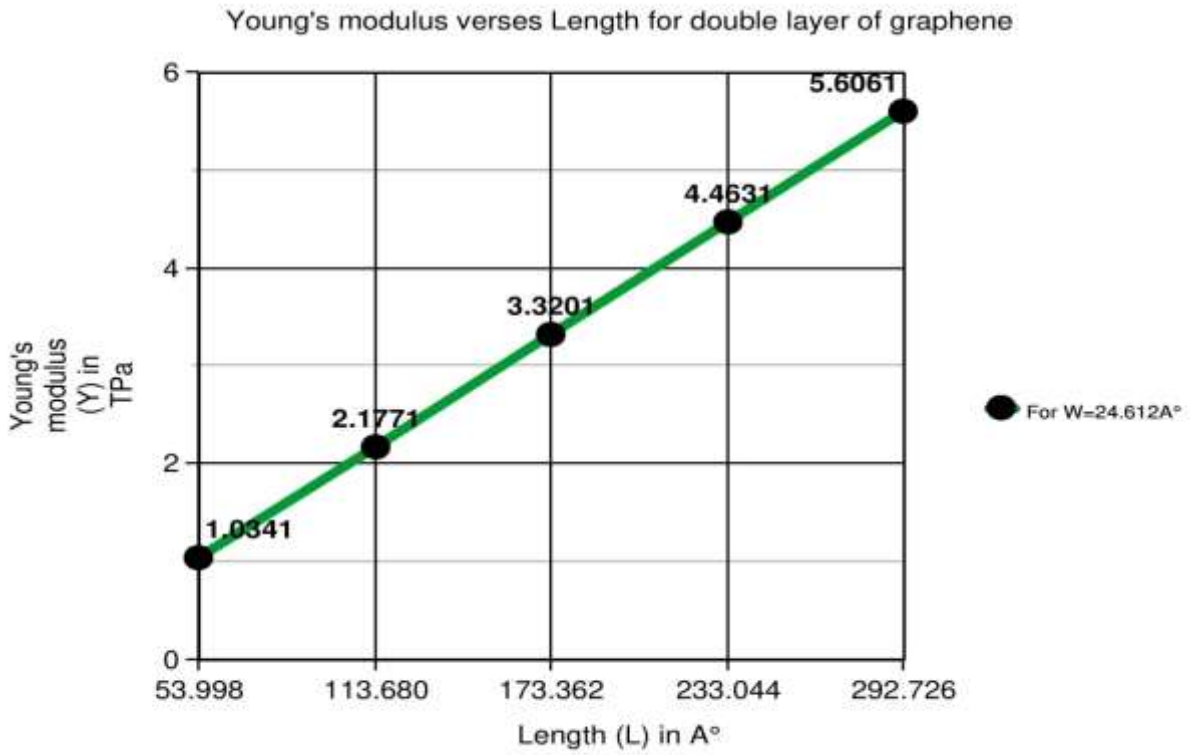

Fig. 3.4 Loading in zigzag direction for double layer of graphene

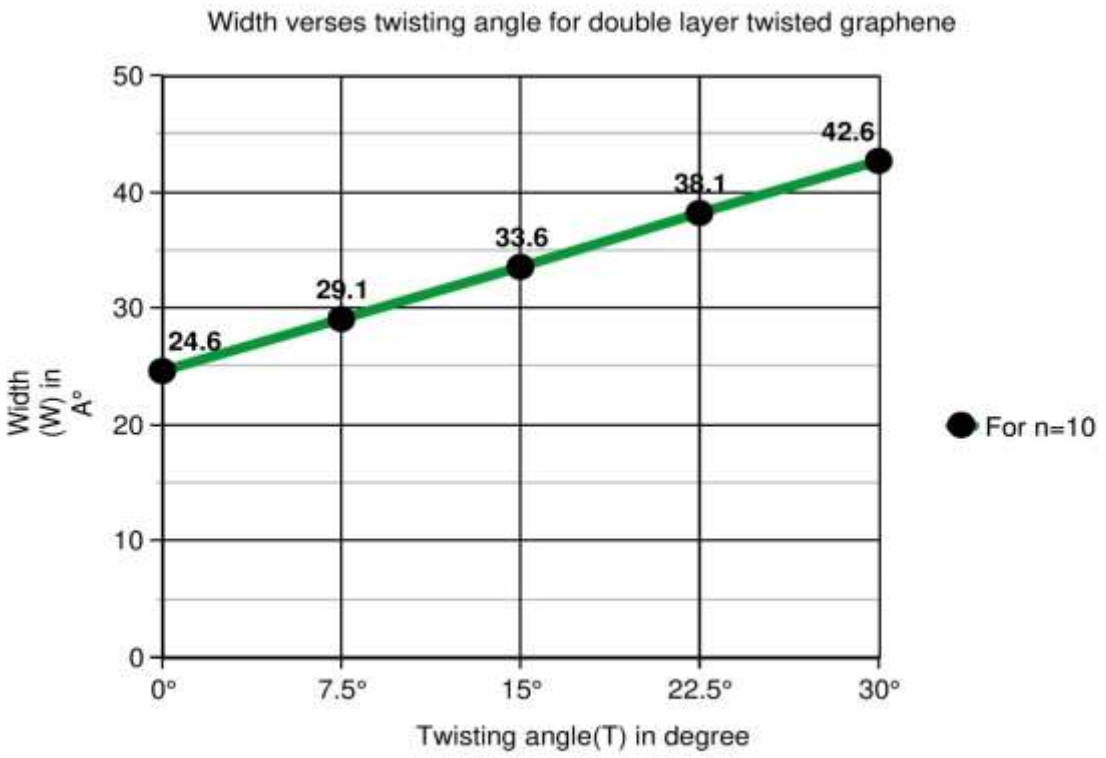

Fig. 3.4(a) Width verses twisting angle for double layer twisted graphene

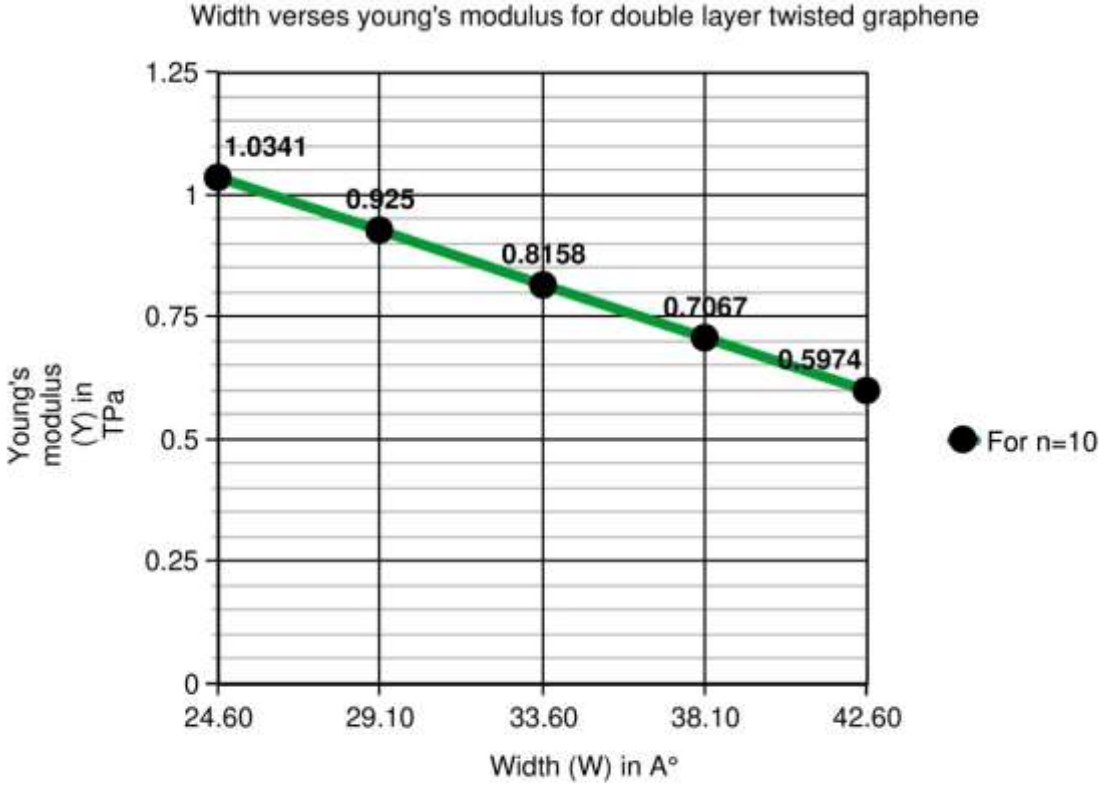

Fig. 3.4(b) Width verses young's modulus for loading in Zigzag direction

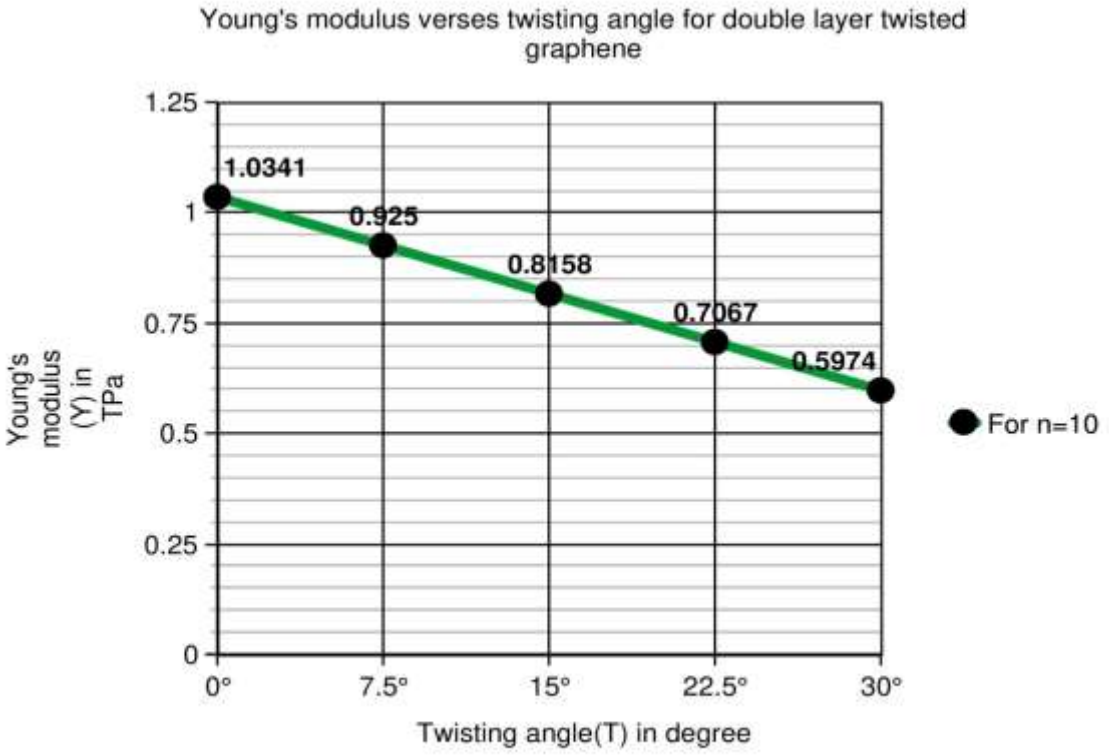

Fig. 3.4(c) Young's modulus verses twisting angle for loading in Zigzag direction

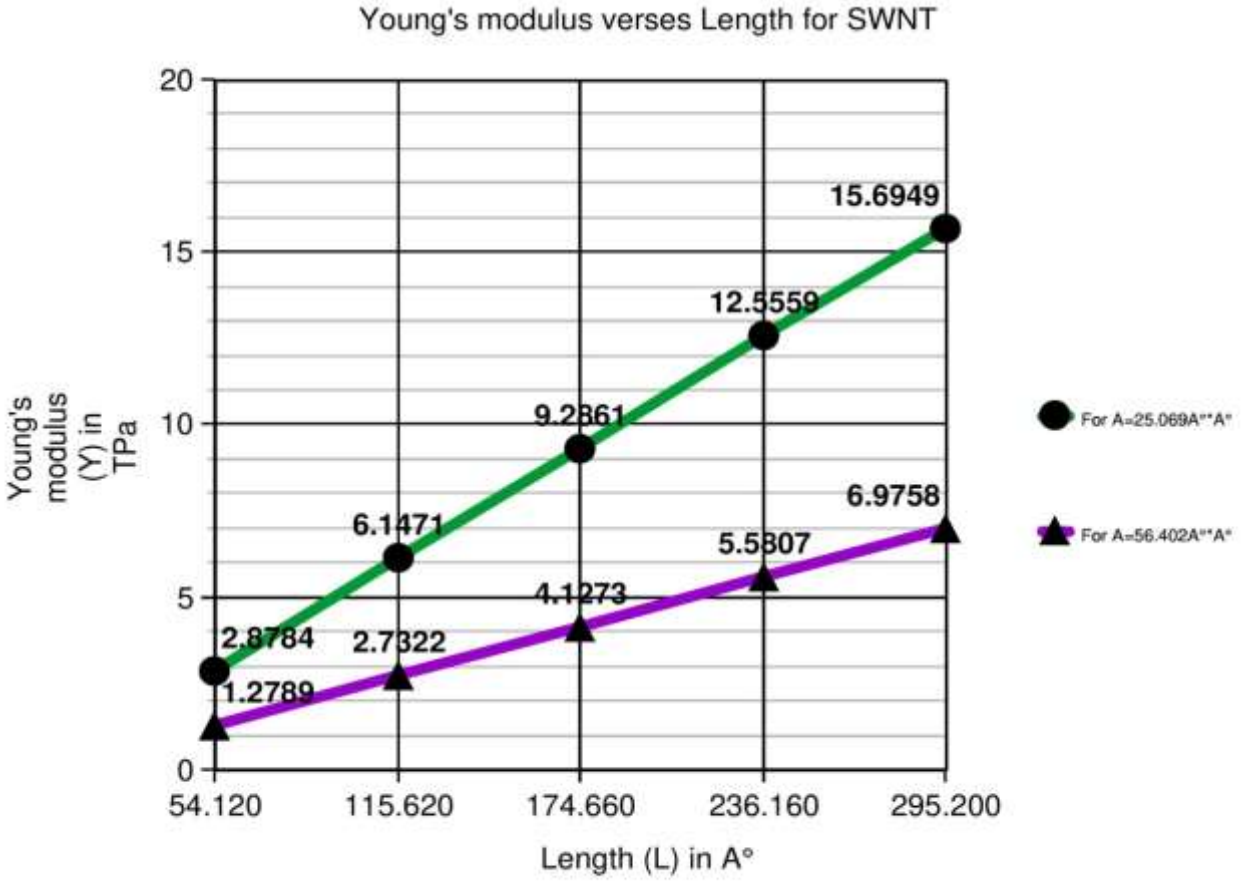

Fig. 3.5 Loading in armchair direction for SWNT

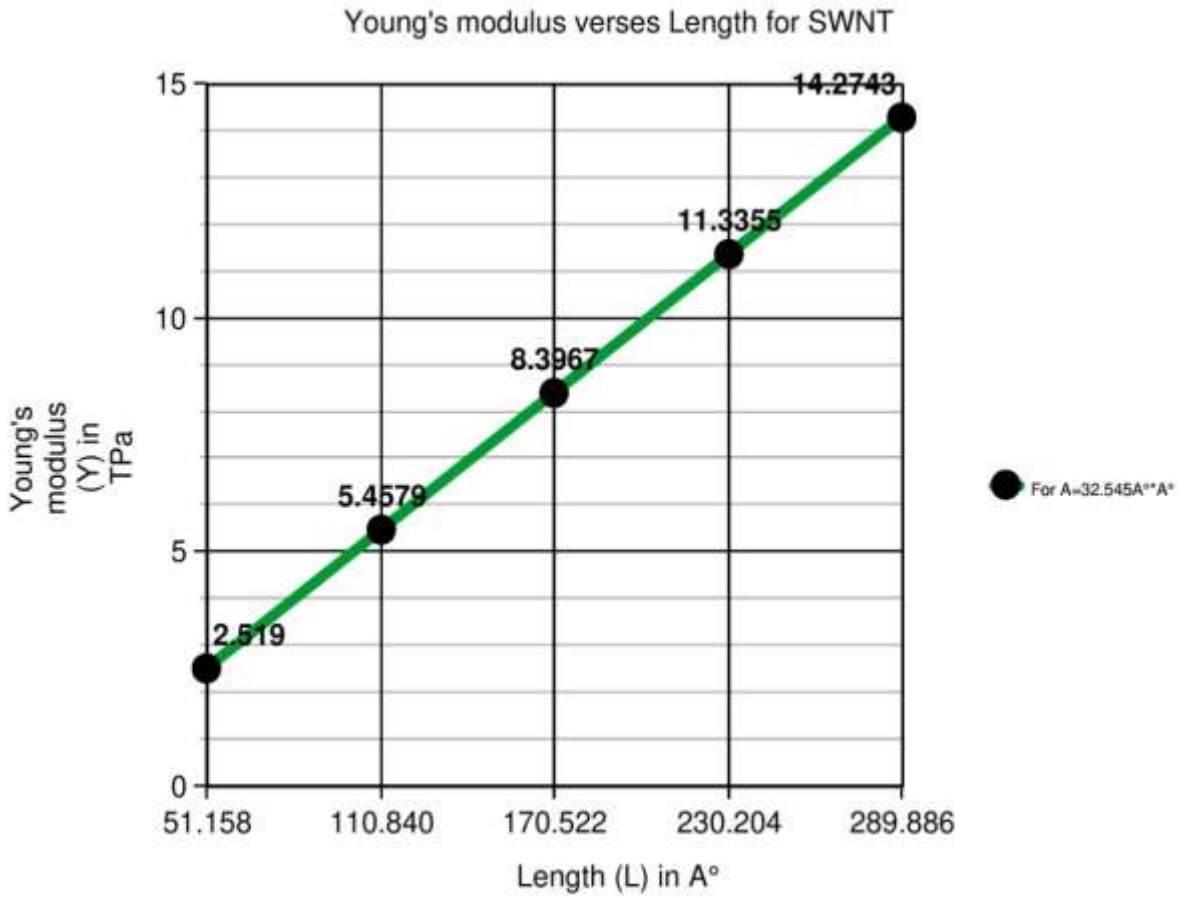

Fig. 3.6 Loading in zigzag direction for SWNT

Hence, Young's modulus of single layer graphene sheet and its derivatives is calculated using equation (1.2) and equation (1.3) for different width and length of the sheet. Firstly a graphene sheet of width W=19.894Å and W=41209Å are taken and load is applied along armchair direction for different length(50Å-300Å).Young's modulus is calculated. The result is plotted in fig. 3.1.From the curve it is clear that young's modulus increases with length of graphene sheet and is in agreement of result of ref.(lengvarsky and bocko,2015). Secondly, graphene sheet of width W=24.612Å is taken and load is applied along zigzag direction for different length (50Å-300Å) of graphene sheet. Young's modulus is calculated. The result is plotted in fig. 3.2. From the curve it is clear that young's modulus increases with length of graphene sheet.

Similarly, we get result for graphene derivatives. Hence, at constant width, Young's modulus increases with length for graphene derivatives. It is clear that young's modulus of single layer of graphene is larger than double layer of graphene. Young's modulus of zigzag direction is larger than armchair direction. In the case of twisting of double layer, we get linearly decrease in young's modulus with twisting angle.

CONCLUSION - At nano scale, we see that young's modulus of graphene and its derivatives depends on physical structure of material. We get different values for different length for particular width and thickness. In present work, expression of young's modulus for nano scale graphene sheet is derived using the fact that it depends on elastic constant. This seems reasonable as when length is increased keeping width constant, young's modulus increases as length of the graphene and its derivatives increases. Young's modulus of single layer of graphene is larger than double layer of graphene. Young's modulus of zigzag direction is larger than armchair direction. In the case of twisting of double layer, we get linearly decrease in young's modulus with twisting angle.

Hence, We can say that work performed in this paper may be very fruitful in the area of nano material and nano science. Equation deduced in this paper as equation (1.4) can open new path to mechanical analysis of nano materials.

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