BILINGUAL PUBLISHING CO.
Pioneer of Global Academics Since 1984

Journal of Mechanical Engineering Research
https://ojs.bilpublishing.com/index.php/jmer

ARTICLE

Geometrical Dimensional Effect on Natural Frequency of Single Layer Graphene in Armchair Configuration

Harshad Patel*

Manufacturing Engineering Department, Central Institute of Petrochemicals Engineering & Technology, Ahmedabad, Gujarat, India

ARTICLE INFO

Article history
Received: 14 October 2021
Revised: 1 November 2021
Accepted: 12 November 2021
Published Online: 18 November 2021

Keywords:
Single layer graphene sheet (SLGS)
Size variation
Fundamental natural frequency
Finite element analysis

ABSTRACT

Graphene has remarkable strength, such as yield strength and elastic constant. The dynamic behaviour of graphene sheet is affected by geometrical variation in atomic arrangement. This paper introduced graphene with armchair atomic structure for estimating fundamental natural frequencies. The presented analysis can be useful for the possible high frequency nanomechanical resonator systems. The analytical formulation, based on classical plate theory and continuum solid modelling based finite element method have been performed for estimation of fundamental natural frequencies of single layer graphene sheet (SGLS) with different boundary conditions. The free edge and clamped edge boundary conditions have been considered. For simplifying analytical formulations, Blevins approach for dynamic solution has been adopted and for validating analytical results. The finite element analysis of SLGS has been performed using ANSYS software. The effect of variation in geometrical parameters in terms of width and length of SLGS has been analysed for realization of ultra-high frequency based nanomechanical resonator systems.

1. Introduction

There are many discoveries for nano structures have been found in which, graphene is the most predominant invention of the engineering science. And till date many broad range of innovation are appraised for exploring the properties such as thermal, electrical, and mechanical of graphene as a nanostructure [1,2]. There are several allotropes, investigated based on carbon in which different phenomenon such as 3-dimensional, 2-dimenionsal and 1-dimensional allotropes were identified as graphite, graphene and nanotube respectively [3-7]. In the structure of graphene, carbon atoms are bonded very densely as honeycomb arrangement with sp2 bond. Graphene has excellent material properties, which attracts the field of application such as nanoelectronic, bio mechanical, nano sensing element, resonators etc [8,9]. In the recent years, grapheme has been placed as stronger material in the field of material engineering due to its stunning material properties such as electrical, thermal, and chemical [10,11]. Properties such as mobility of electron at room temperature as 250000 cm^2/Vs, thermal conductivity 5000 W/mK [12], explored surface area as 2630 m^2/g [13] made it versatile in the today's era.

Numerous researches on single layer graphene sheet have been done, which employ static and dynamic phenomenon such as static behaviors, fatigue and vibration

**Corresponding Author:*
Harshad Patel,
Manufacturing Engineering Department, Central Institute of Petrochemicals Engineering & Technology, Ahmedabad, Gujarat, India;
Email: patel.harshad0585@gmail.com

 DOI: https://doi.org/10.30564/jmer.v4i2.3831

behaviors. [14,15]. For example, Sakhaee et al. [16] had performed molecular structural mechanics and reported that single layer graphene sheet has remarkable dynamic behaviors. There are many technical phenomenon are completed on graphene for cultivating comprehension of behaviors of graphene with different boundary conditions such as clamped-pinned with mass, Clamped-pinned without mass etc [17]. Moreover, there are many technical aspects which are not explored yet by researchers in the field of material engineering that can distinguish the dynamic approach. Various boundary conditions and support conditions with different theories such as molecular dynamic theory, computational approaches etc. are still in consideration for investigation [18,19].

Graphene has principal applications in the field of biomechanical as sensor or in nanomechanical system as mass sensor [20]. The system based on graphene may have higher sensitivity as a mass sensor for monitoring resonance frequency. In the structural applications, aeronautical applications, automobile sectors, there are various aspects of graphene or graphene based composite material utilization, which can add noticeable advantages in terms of static and dynamic strength [21]. The atomic structures of graphene can be classified as armchair, zigzag and chiral and different types atomic structure of graphene affect significantly to the graphene's behaviors in static and dynamic condition. In the armchair atomic structure, at the free edges along width of graphene sheet carbon-carbon bond of each hexagon are parallel to lateral dimensions as width of graphene sheet. When large portion of graphene is cut along sides of hexagons, then armchair structure is obtained [22]. In the zigzag atomic structure, at the free edges along width of graphene sheet carbon-carbon bond of each hexagon are 60 degrees offset to the axis of width of graphene sheet. When large graphene sheet is cut along sides the vertices of hexagons, then zigzag structure is obtained [22,23].

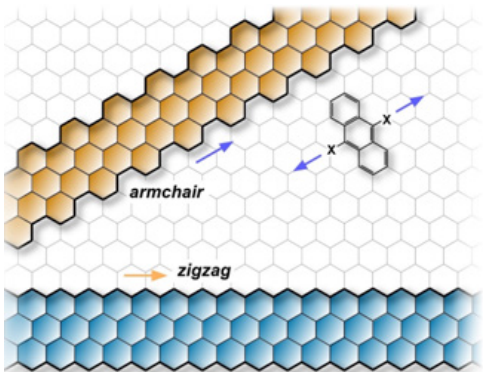

Figure 1. Direction of cutting graphene sheet to obtain armchair and zigzag structure [22]

2. Analysis Approach

In this research work, graphene sheet is simulated by employing three different approaches said, analytical, finite element analysis, and space frame modeling approach. The analytical approach has been employed for obtaining results based on analytical formulations, the obtained results are validated using continuum modeling based finite element analysis using ANSYS workbench.

2.1 Analytical Approach

The analytical formulation of the graphene sheet with armchair configuration has been performed by considering graphene sheet as a rectangular plate like structure. The classical plate theory based on Kirchoff theory for thin plate has been applied on the graphene sheet. Assumption further extended towards single layer of rectangular plate; as graphene sheet is a two-dimensional atomic structure. The thickness has been considered as diameter of carbon atom. The equation of motion has been derived by employing equilibrium approach of solution. And, the natural frequencies are obtained based on Blevins solution for dynamic approach.

There are two motions in the concept of vibration phenomenon, which are important to technical point of view; known as transverse and longitudinal, and both are to be considered for understanding deformation in each direction. Deformation in specific direction decides stress level in particular direction as per boundary and support conditions so fundamental mode shape with natural frequency is become an important aspect of study. In this study, analytical calculation is executed by considering transverse direction only and Blevins solution of natural frequency is employed. As per equilibrium approach, equation of motion can be derived as,

$$D\left(\frac{\partial^4 w}{\partial^4 x}+2\,\frac{\partial^4 w}{\partial^2 x*\partial^2 y}+\frac{\partial^4 w}{\partial^4 y}\right)+\rho h\frac{\partial^2 w}{\partial t^2}=0 \qquad (1)$$

Now, considering no deformation at two adjacent sides, x = 0, y = 0. And considering free vibration, i.e. force = 0, solution of equation (1) is given by,

$$W(x,y) = a1\,\sin\alpha x\,\sin\beta y + a2\,\sin\alpha x\,\cos\beta y + a4\,\cos\alpha x\,\cos\beta y + a5\,\sinh\theta x\,\sinh\emptyset y + a6\,\sinh\theta x\,\cosh\emptyset y + a7\,\cosh\theta x\,\sinh\emptyset y + a8\,\cosh\theta x\,\cosh\emptyset y$$

Where, $\lambda 2 = \alpha 2 + \beta 2 = \theta 2 + \emptyset 2$

Blevins had derived various dynamic solutions considering numerous boundary conditions such as bridge boundary, cantilever boundary condition etc. Bridge boundary condition is set by clamping two opposite edges and by keeping two free edges whereas cantilever has

DOI: https://doi.org/10.30564/jmer.v4i2.3831

one clamped edge and three free edges [24,25]. Based on mentioned boundary conditions, Blevins had developed various constants as per mode index, which are mentioned below,

$$\omega_{ij} = \sqrt{\left\{\frac{\pi^4 F}{a^4 h\rho}\right\}\left\{H_x{}^4 + H_y{}^4\left(\frac{a}{b}\right)^4 + 2\left(\frac{a}{b}\right)^4\left[\vartheta J_x J_y + (1-\vartheta)K_x K_y\right]\right\}} \quad (2)$$

Where, $F, Flexural\ Density = \frac{Eh^3}{12(1-\vartheta^2)}$

H*x, Jx, Kx, Hy, Jy, Ky*; all are constants depend on boundary conditions.

Table 1. Edges along Length (Free-Free boundary)

Mode index (j)	Hy	Jy	Ky
1	0	0	0
2	0	0	1.22
3	1.51	1.25	5.017

Table 2. Edges along Length (Clamped-Clamped boundary)

Mode index (j)	Hx	Jx	Kx
1	1.51	1.29	1.25
2	2.5	4.658	4.658
3	3.5	10.02	10.02

Table 3. Edges along Length (Clamped-Free boundary)

Mode index (j)	Hx	Jx	Kx
1	0.597	-0.0870	0.471
2	1.494	1.347	3.284
3	2.5	4.658	7.842

Consider (5,5) armchair configuration for length 10A of the graphene.

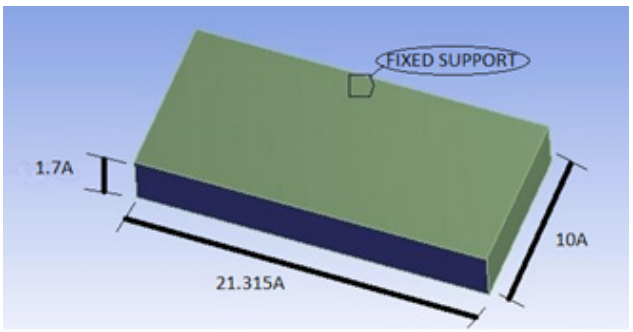

Figure 2. General Dimensions of the Model

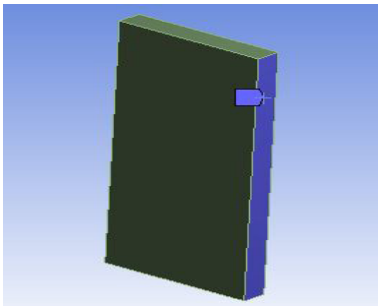

Figure 3. Free-Free-Free-Clamp (F-F-F-C) Boundary Condition (FEM)

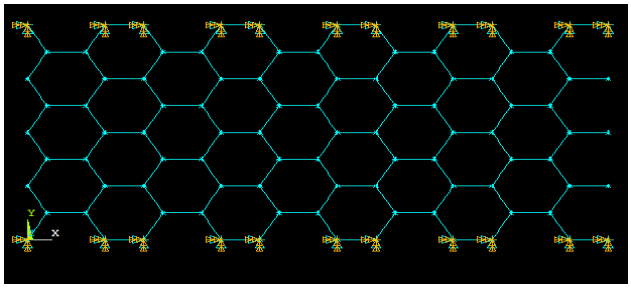

Figure 4. Free-Free-Clamp-Clamp (F-F-C-C) Boundary Condition (SFA)

In general, two major boundary conditions are considered such as bridge boundary condition and cantilever boundary conditions. Bridge boundary condition is defined as Free-Free-Clamp-Clamp (F-F-C-C) whereas cantilever boundary condition is defined as Free-Free-Free-Clamp (F-F-F-C). In bridge boundary condition opposite sides of the Graphene was fixed and two sides are remaining free whereas in cantilever boundary condition three sides of the Graphene remain free and one is fixed.

This concept is applied to all three approaches, numerical, finite element analysis and finite element analysis (Space Frame Analysis). In numerical approach, boundary conditions with constants are presented in Table 1, 2 & 3 through which analytical calculation is carried out for all armchair dimensions whereas FEA and FEA (SFA) are presented as per the below models created in ANSYS modeler and ANSYS APDL.

Now from above tables, constants for bridge boundary condition are decided as,

ω_{11} *as* Hx = 1.506, Jx = 1.248, Kx = 1.248,
Hy = 0, Jy = 0, Ky = 0
ω_{12} *as* Hx = 2.5, Jx = 4.658, Kx = 4.658, Hy = 0,
Jy = 0, Ky = 0

The one of the basic calculations of (5,5) armchair patter of graphene is derived here as,

DOI: https://doi.org/10.30564/jmer.v4i2.3831

$$\text{Flexural rigidity (F)} = \frac{E*h^3}{12*(1-\vartheta^2)} = \frac{10^{12}\times(3.45\times10^{-10})^3}{12(1-0.456^2)}$$

$$= 4.320 * 10^{-18}\text{N.m}$$

$$\omega_{11} = \sqrt{\left\{\frac{\pi^4*4.3203*10^{-18}}{(10^{-9})^4*1161*1.7*10-10}\right\}\left\{\begin{matrix}1.506^4 + 0^4\left(\frac{1}{2.1315^1}\right)^4 + 2\left(\frac{1}{2.1315^1}\right)^4 \\ \times [0.456 * 1.248 * 0 + (1 - 0.456)1.248 * 0]\end{matrix}\right\}}$$

$$= 6.62*10^{12}\text{Hz}$$

$$\omega_{12} = \sqrt{\left\{\frac{\pi^4*4.3203*10^{-18}}{(10^{-9})^4*1161*1.7*10-10}\right\}\left\{\begin{matrix}2.5^4 + 0^4\left(\frac{1}{2.1315^1}\right)^4 + 2\left(\frac{1}{2.1315^1}\right)^4 \\ \times [0.456 * 4.658 * 0 + (1 - 0.456)1.248 * 0]\end{matrix}\right\}}$$

$$= 6.73*10^{12}\text{ Hz}$$

2.2 Finite Element Analysis

Continuum finite element method based approach of graphene sheet has been performed in ANSYS workbench for various configuration such as (11,11), (15,15), and (19,19). All the configuration are simulated using ANSYS workbench with bridge and cantilever boundary conditions. Dimensions of graphene sheet configuration was set as 10 x 21.31 Å with thickness of graphene as 170 Å which is diameter of carbon atom. For continuum solid modeling based finite element analysis approach, all the configurations have been simulated as per bridge and cantilever boundary conditions with different length of graphene sheet.

Table 4. Properties of Graphene.

Sr. No.	Property	Value
1	Poisons ratio u	0.456
2	Density ρ	1161Kg/m^3
3	Young's modulus E	1 TPa=10^{12} Pa

Table 5. Geometrical Dimension of Graphene.

Sr. No.	Dimensions	Value
1	length of graphene sheet, *a*	10A =10^{-9} m
2	Width, *b*	21.315A=2.1315 x10^{-9} m
3	Thickness	0.17nm =1.7 x10^{-10} m

2.3 Space Frame Approach (FEA)

Space frame approach is advanced version of FEM based nodal calculation and for getting the advantage of this, ANSYS APDL is employed in the analysis. In ANSYS APDL all the coordinated are deployed from the Nano modeler software and file is exported in ANSYS APDL.Graphene sheet has hexagonal arrangement of atoms such as honey comb structure [26,27]. Results obtained, using continuum solid modeling approach has been validated by performing space frame modeling approach using ANSYS APDL. The development of space frame model of graphene sheet in ANSYS APDL requires the co-ordinates of all the atoms of carbon to represent approximation of single layer graphene sheet. The space frame models of (11,11) configuration has shown in Figure 3, which is developed using ANSYS APDL. Similarly, the space frame model of atomic structures (15,15) and (19,19) have been developed.

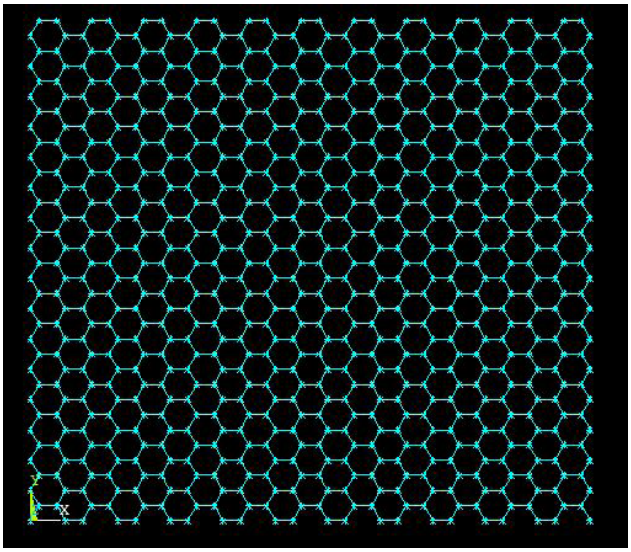

Figure 5. Space Frame of (11, 11) configuration

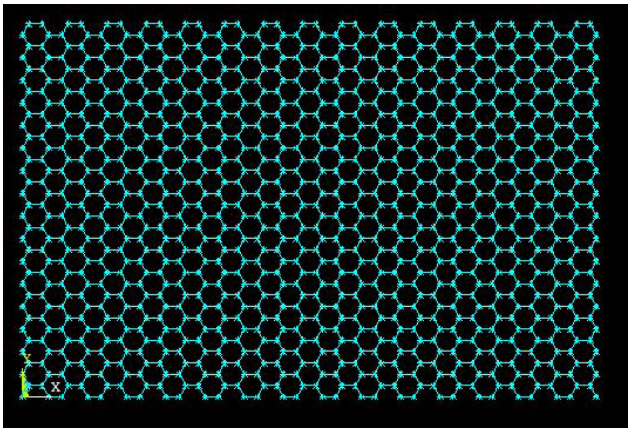

Figure 6. Space Frame of (15, 15) configuration

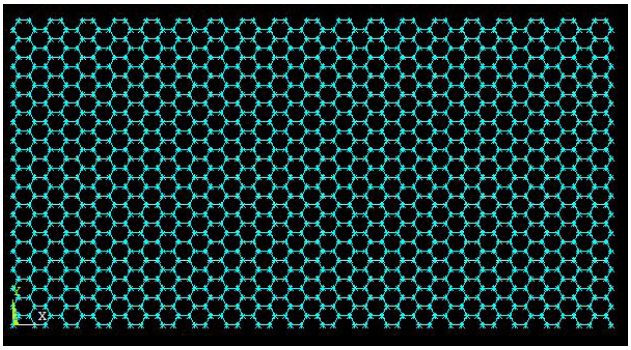

Figure 7. Space Frame of (19, 19) configuration

DOI: https://doi.org/10.30564/jmer.v4i2.3831

3. Results & Discussion

Single layer graphene sheet has been analyzed by three approaches as, analytically, finite element analysis, and finite element analysis with space frame approach. The analysis has been performed with different lengths of the graphene as 41.21A, 83.83A, 126.46A, 169.08A, and 211.71A, for three different widths of 12.31A, 17.23A, and 22.15A of the graphene sheet. The obtained results for bridged and cantilevered configurations are summarised in Table 6 and Table 7 respectively for all the considered approaches.

Table 6. Comparison of Natural Frequency (Bridge Boundary Condition)

Configuration (Armchair)	Width	Length	Analytical (GHz)	FEA (GHz)	FEA(SFA) (GHz)
(11,11)	12.31A	41.21A	669	599	600
		83.83A	162	147	154
		126.46A	71	64.5	66.1
		169.08A	39.7	36.0	38.1
		211.71A	25.3	22.9	24.1
(15,15)	17.23A	41.21A	668	607	632
		83.83A	160	149	158
		126.46A	70	65.2	70.4
		169.08A	39	36.3	38.0
		211.71A	25	23.1	23.9
(19,19)	22.15A	41.21A	665	612	655
		83.83A	158	150	162
		126.46A	68	65.7	68.9
		169.08A	39	36.6	38.7
		211.71A	25	23.2	30.0

Table 7. Comparison of Natural Frequency (Cantilever Boundary Condition)

Configuration (Armchair)	Width	Length	Analytical (GHz)	FEA (GHz)	FEA(SFA) (GHz)
(11,11)	12.31A	41.21A	105	96.1	93.0
		83.83A	25.4	23.0	24.2
		126.46A	11.2	10.1	10.6
		169.08A	6.24	5.61	5.96
		211.71A	3.98	3.57	3.20
(15,15)	17.23A	41.21A	106	97.4	98.0
		83.83A	25.9	23.2	24.9
		126.46A	12.0	10.1	9.10
		169.08A	6.52	5.64	5.50
		211.71A	4.10	3.59	3.91
(19,19)	22.15A	41.21A	106.5	98.5	106
		83.83A	26.0	23.3	29.8
		126.46A	12.1	10.2	10.4
		169.08A	6.72	5.66	6.60
		211.71A	4.19	3.60	4.25

3.1 Bridge Boundary Condition

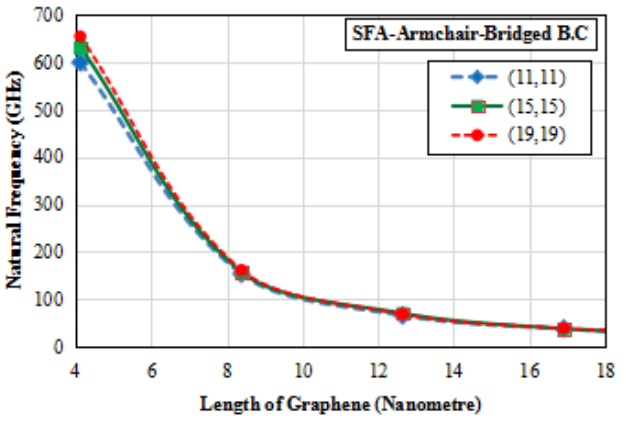

Figure 8. Variation of Natural Frequency in Bridged Boundary Condition

In armchair atomic configuration of graphene sheet, for bridge boundary condition obtained results shows that, the maximum natural frequency for (19, 19) is 655 GHz, whereas for (11, 11) armchair configuration the maximum natural frequency is 601 GHz. From Figure 8, it has been observed that, as the length of graphene sheet increases the natural frequencies decreases irrespective of configuration of (19, 19), (15,15), and (11,11).

3.2 Cantilever Boundary Condition

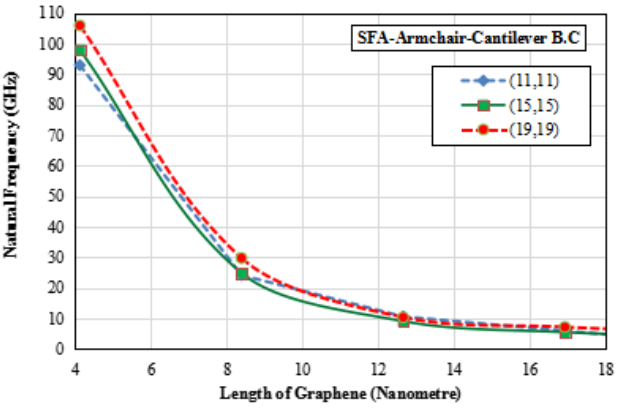

Figure 9. Variation of Natural Frequency in Cantilever Boundary Condition

For cantilevered configuration obtained results (Table 7) also depicts that as the length of graphene sheet increases the natural frequency decreases irrespective of different considered armchair configurations. Also, it has been observed that for the same size frequency of graphene sheet for bridged boundary condition is higher than that for the cantilevered boundary condition (Figure 9). Such results suggest that cantilevered boundary condition is more sensitive than that of bridged boundary condition.

DOI: https://doi.org/10.30564/jmer.v4i2.3831

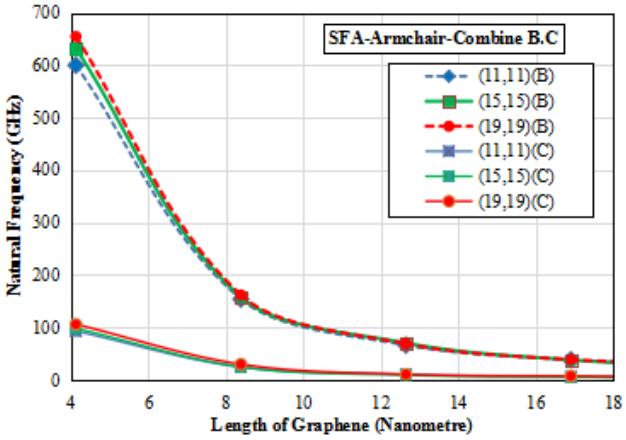

Figure 10. Variation of Natural Frequency in Bridged & Cantilever Boundary Condition

4. Conclusions

The present research work on Graphene was introduced for identification of dynamic behaviours based on analysis of natural frequency variation. Size variation of graphene sheet is carried out by performing modal analysis in finite element analysis and FEA space frame approach in ANSYS APDL and found to be useful for further realization of ultra-high frequency nanomechanical resonators. The present analysis also suggests that as the size of the graphene sheet increases (either width or length) the natural frequencies of graphene sheet decreases. Also, it has been observed that for a particular size of graphene sheet the natural frequency is found higher for bridged boundary condition compared to cantilevered boundary condition in armchair configuration. Such results depict that cantilevered boundary condition is found more sensitive compared to bridged boundary condition the armchair configuration. It has been observed that outcome from the research work is resembled in all analysis domains such as numerical, finite element method, and finite element analysis in space frame approach for natural frequency so the reliability of the space frame approach and finite element analysis can be carried out to nano size of the plate said as for Graphene. The presented analysis is found to be useful for the realization of high frequency sensor system based on nanomechanical resonator, which can be utilized as a mass sensor, gas-sensor, bio-detection sensor system etc.

References

[1] S. Iijima // *Nature* 354 (6348) (1991) 56.
[2] K. Esumi, M. Ishigami, A. Nakajima, K. Sawada, H. Honda // *Carbon* 34 (1996) 279.
[3] F. Scarpa, S. Adhikari, A. Srikantha Phani // *Nanotechnology* 20(6) (2009) 065709.
[4] K. Tanaka, H. Aoki, H. Ago, T. Yamabe, K. Okahara // *Carbon* 35 (1997) 121.
[5] M. Kim, H.S. An, W.-J. Lee, J. Jung // *Electronic Materials Letters* 9(4) (2013) 517.
[6] M. Mazar Atabaki, R. Kovacevic // *Electronic Materials Letters* 9(2) (2013) 133.
[7] W.G. Lee, E. Kim, J. Jung // *Electronic Materials Letters* 8(6) (2012) 609.
[8] C. Berger, Z. Song, T. Li, X. Li, A.Y. Ogbazghi, R. Feng, Z. Dai, A.N. Marchenkov, E.H. Conrad, P.N. First, W.A. de Heer // *The Journal of Physical Chemistry B* 108(52) (2004) 19912.
[9] J.S. Bunch, A.M. Van Der Zande, S.S. Verbridge, I.W. Frank, D.M. Tanenbaum, J.M. Parpia, H.G. Craighead, P.L. McEuen // *Science* 315 (2007) 490.
[10] S.S. Gupta, R.C. Batra, Journal of Computational and Theoretical Nanoscience 7 (10) (2010) 2151-2164.
[11] S. Timoshenko, Theory of Plates and Shells, McGraw-Hill, Inc, London, 1940.
[12] Balandin AA, Ghosh S, Bao W, Calizon I, Teweldebrhan D, Miao F, et al. Superior thermal conductivity og single-layer graphene. Nano Lett 2008;8(3):902-7.
[13] Zhu Y, Murali S, Cai W, Li , Suk JW, Potts JR, et al. Graphene and graphene oxide: synthesis, properties, and application. Adc Mater 2010;22(35):3906-24.
[14] Jena, Subrat & Chakraverty, S.. (2019). Dynamic Analysis of Single-Layered Graphene Nano-Ribbons (SLGNRs) with Variable Cross-Section Resting on Elastic Foundation. Curved and Layered Structures. 6. 132-145. 10.1515/cls-2019-0011.
[15] Ren Wei Jiang, Zhi Bin Shen, Guo Jin Tang, Vibration analysis of a single-layered graphene sheet-based mass sensor using the Galerkin strip distributed transfer function method, 2016.
[16] A. Sakhaee-Pour, M.T. Ahmadian, A. Vafai // *Solid State Communications* 145 (2008) 168.
[17] Laura, P.A.A.; Pombo, J. L.; Susemihl, E.A. A note on the vibration of a clamped free beam with a mass at the free end. J. Sound Vib. 1974, 37, 161-168.
[18] Natsuki, Toshiaki. (2015). Theoretical Analysis of Vibration Frequency of Graphene Sheets Used as Nanomechanical Mass Sensor. Electronics. 4. 723-738. 10.3390/electronics4040723.
[19] Samaei, A.T. & Aliha, M.R.M. & Mirsayar, M.M.. (2015). Frequency analysis of a graphene sheet embedded in an elastic medium with consideration of small scale. Materials Physics and Mechanics. 22. 125-135.
[20] Ekinci, K.L.; Huang, X.M.H.; Roukes, M.L. Ultrasensitive nanoelectromechanical mass detection.

DOI: https://doi.org/10.30564/jmer.v4i2.3831

Appl. Phys. Lett. 2004, 84, 4469-4471.
[21] Geim, A.K. Graphene: status and prospects. Science 2009, 324, 1530-1534.
[22] Rakesh Prabhu T., Tarapada Roy, National Institute Of Technology ROURKELA,2010.Finite element modelling of multiwall carbon nanotube.
[23] Steven J. Koester ,Ultra-smooth Graphene Nanoribbon Formation Using Templated,Etching.
[24] Blevins, R. Formula for Natural Frequency and Mode Shape; Krieger; Hellerup, Denmark, 2001.
[25] Belvins, R.D. (1984) Formulas for natural frequency and mode shape. R.E. Krieger.
[26] Rakesh Prabhu T., Tarapada Roy, "Finite element modeling of multiwalled carbon nanotube". National Institute of Technology Rourkela,2010.
[27] Zenkour, Ashraf. (2016). Vibration analysis of a single-layered graphene sheet embedded in visco-Pasternak's medium using nonlocal elasticity theory. Journal of Vibroengineering. 18. 10.21595/jve.2016.16585.

 DOI: https://doi.org/10.30564/jmer.v4i2.3831