Impact of Defects on Critical Buckling Load of a Single-Layer Nanoplate with Various Plate Aspect Ratios

R VITTAL[1], CHANDRAPPA S [2], SMITHA T K [3]
[1] Senior *Scale Lecturer, Department of Mechanical Engineering, Government polytechnic Mulabagal, Karnataka, India.*
[2] Lecturer, *Department of Mechanical Engineering, Government polytechnic K.G.F, Karnataka, India.*
[3] Senior *Scale* Lecturer, *Department of Automobile Engineering, S J (Government) polytechnic Bengaluru, Karnataka, India.*

Abstract: **This study explores the buckling behavior of single-layer armature-type graphene nanoplates of differing sizes, focusing on the influence of atomic vacancy defects with varying distributions. This study presents a unique perspective by comprehensively exploring the impact of various factors that have not been extensively addressed in earlier research. These factors include aspect ratio, defect concentration, and different boundary conditions such as clamped-free (CF), clamped-clamped (CC), and simply-supported (SS), all of which play a significant role in the buckling behavior of graphene nanoplates. In order to preserve the unique attributes of the nanoplates, an innovative approach was employed to characterize them through the use of space frame structures. The buckling behavior was anticipated through the application of the finite element method (FEM). The simulation findings for the critical buckling load (*Pcr*) were validated through a careful comparison with relevant data available in the open literature. The results indicate that *Pcr* experiences a significant decrease at lower aspect ratios when this factor is diminished, though this reduction appears to become more gradual as the aspect ratios increase. Moreover, it has been demonstrated that atomic-scale imperfections notably reduced *Pcr*; for instance, a 10% concentration of defects led to an approximate 40% reduction in the critical buckling load, highlighting the significant influence that defects exert on the stability of nanostructures.**

Keywords: **Aspect Ratios; Layers; Buckling load; Defects.**

1. INTRODUCTION AND LITERATURE ASSESSMENT

Recent developments in the research of nanoplates, characterized by their two-dimensional nanoscale structures, have generated a notable interest. Due to their remarkable characteristics and extensive range of potential applications, both single-layer and multilayer graphene sheets have garnered significant attention in research endeavors [1,2].

Due to its remarkable mechanical, electrical, and thermal characteristics, graphene—the strongest and thinnest material known—has garnered significant interest. The unique properties of graphene nanoplates render them appealing choices for various applications across multiple sectors, such as biomedical technologies, solar energy systems, transistors, electromechanical devices, nanosensors, and nanoactuators. The potential of these materials to transform the electronics, energy storage, and healthcare sectors is significant. Consequently, extensive theoretical and experimental research is being conducted to explore their behavior under various operating conditions. The initial series of theoretical investigations employs the finite element method (FEM) alongside computational techniques, drawing from the perspectives of atomic, continuum, and molecular mechanics. While each of these approaches presents its own advantages and disadvantages, numerous researchers have employed them to explore different aspects of nanostructures, particularly graphene. The mechanical behavior of single-layer graphene sheets has been thoroughly examined through atomic-based techniques such as density functional theory, tight-binding, and molecular dynamics (MD) [9]. Numerous researchers have conducted examinations of the mechanical behavior of graphene sheets, focusing on aspects such as ultimate strength, Young's modulus, and the variations in Young's modulus and shear modulus across different temperatures, employing molecular dynamics simulations as their primary method. Wang and Zhang have recently

conducted a study on the Young's modulus and fracture toughness of bilayer graphene through molecular dynamics simulations. Their findings indicate that while temperature exerts minimal influence on the elastic modulus, it plays a significant role in determining fracture toughness [10]. In another study, Wang et al. examined the shortcomings of imperfect graphene characterized by vacancies and Stone-Wales (S-W) defects. [11]. Through MD simulations, Fadaei Heydari et al. [12] explored the influence of graphene oxide nanoparticles (GO-NP) on the mechanical and thermal properties of PU/PCL nanocomposites. The findings indicated that an ideal equilibrium was attained at a 2% GO-NP concentration, enhancing mechanical strength, heat flux, and thermal conductivity while preserving the material's inherent qualities.

The continuum-based technique, which adeptly captures the distinctive features of small-scale structures, serves as the cornerstone of the second theoretical approach. The approach employed by Behfar and Naghdabadi was aimed at exploring the vibration characteristics of multilayer graphene sheets situated within an elastic medium [13]. Another paper also presented an analytical method for predicting the flexural modulus of multilayer graphene sheets [14]. A continuum-plate model was developed by Kitipornchai et al. [15] to examine the vibrations of multilayer graphene sheets.

Jafari et al. [16] conducted an investigation into the free vibration behavior of nanoplates by employing a combination of classical and non-classical theories, including the implicit gradient, non-local differential form, first-order strain gradient, and second-order strain gradient. The study involved a thorough evaluation of various characteristics, such as classical and nonlocal properties, boundary conditions, and plate dimensions. This was achieved through a numerical solution of partial differential equations, leading to the determination of parametric responses for natural frequencies utilizing the Navier and Galerkin methods. Additionally, Namin and Pilafkan [17] explored the vibrational characteristics of defective graphene sheets through the lens of nonlocal elasticity theory, revealing that atomic structural defects contribute to a decrease in the natural frequencies of these sheets.

The limitations associated with atomic and continuum-based simulations have led to the emergence of a third theoretical perspective, as well as the development of multiscale computing methodologies. Through the integration of molecular mechanics and finite element methods (FEM), these approaches yield atomic-scale FEM models that effectively capture force fields, atomic interactions, and nanoscale phenomena, all while circumventing the necessity for conventional FEM approximations. This approach offers a more cost-effective alternative to molecular dynamics simulations, facilitating the assessment of the buckling force, natural frequencies, and vibration modes of carbon nanostructures [18, 19].

The atomic finite element technique (AFEM) was initially introduced by Liu et al. [20], and its application was later broadened to investigate the mechanical properties of single-walled carbon nanotubes [21]. Gu et al. presented their strain energy curves through the application of AFEM to investigate local buckling in bent single-walled carbon nanotube models [22]. In a similar vein, Pradhan [23] explored the influence of nanoscale factors on the critical buckling stress of single-layer graphene. The findings indicated that buckling ratios increased with higher nonlocal parameter values, while a decrease was observed with longer graphene sheet lengths. To elucidate the characteristics of single-layer graphene sheets and assess their buckling behavior within an elastic medium, Samaei et al. [24] employed nonlocal Mindlin plate theory. Zhang et al. [25] conducted an investigation into the buckling behavior of single-layer graphene sheets within elastic environments, employing the element-free Kp-Ritz technique alongside non-local elasticity theory. Their study emphasizes the significance of surrounding elastic support and nonlocal factors in influencing critical buckling patterns. In the interim, Sakhaee-Pour [26] employed molecular structural mechanics to investigate elastic buckling and identified a nonlinear relationship between buckling force and sheet width, noting that aspect ratio appeared to have no significant effect.

2. FEM SIMULATIONS

The numerical simulations are conducted utilizing a combination of ANSYS and MATLAB. In order to achieve this, the appropriate MATLAB algorithms were developed to construct the model geometry, followed by the importation of data into ANSYS for the execution of the solution and the application of boundary conditions. Furthermore, a MATLAB script was developed to generate a command code that is subsequently executed in ANSYS. As

illustrated in Fig. 1, the model presents a two-dimensional structure characterized by its length a and breadth b, alongside the coordinate system currently in use. The initial phase of the modeling technique involves identifying points that symbolize carbon atoms. The points are subsequently linked by lines that signify covalent bonds. A singular unit cell is established and replicated along the $x-$ and $y-$axes, resulting in the formation of a planar structure that constitutes a complete two-dimensional lattice.

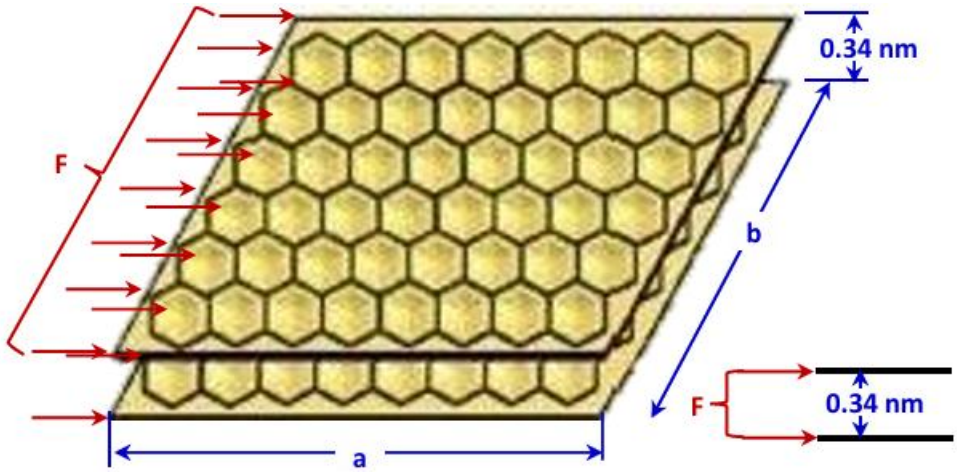

Fig. 1. Interlayer distance in double-layer graphene nanoplates under compression load causing buckling.

The three-dimensional BEAM4 elastic element was employed to articulate the covalent bonds present within the graphene structure. This model incorporates three translational degrees of freedom along the x, y, and z axes, as well as three rotational degrees of freedom around these axes for each node. To effectively illustrate the van der Waals interactions occurring between adjacent layers, interlayer springs were incorporated as well. Interactions were considered solely when the interatomic distance was at or below the cutoff radius, denoted by σ, which is the Lennard-Jones parameter. Atoms were regarded as lacking any interaction beyond this level. The stiffness values of the springs were ascertained through an equivalency method that linked the elastic energy of the springs to the chemical bond energy, following their specification between atomic sites.

A variety of nanoplates, characterized by two distinct width measurements of 30 Å and 70 Å, along with varying lengths, were analyzed to investigate their buckling behavior. In order to facilitate the exploration of the influence of the aspect ratio, a/b, nanoplates of differing lengths were developed corresponding to each width. Additionally, various vacancy concentrations were incorporated into the nanoplate's structure to illustrate the influence of atomic defects on its buckling capacity. Given that boundary conditions play a crucial role in influencing buckling behavior, the diverse types outlined in Table 1 were incorporated into the simulations. The abbreviations CF, CC, and SS represent clamped-free, clamped-clamped, and simply supported boundary conditions, respectively, for the purpose of brevity.

3. APPLIED BOUNDARY CONDITIONS

Table 1 Different applied boundary conditions in buckling analysis

Nanoplate face	Clamped-Free	Clamped-Clamped	Simply-Simply
$y = 0$	$All\ DOF = 0$	$All\ DOF = 0$	$u_x = 0;\ u_y = 0;\ u_z = 0$
$y = a$	$F_y = P$	$u_x = 0;\ u_z = 0; F_y = P$ $All\ rotation = 0$	$u_x = 0;\ u_z = 0;\ F_y = P$

4. VALIDATION

A comparison has been conducted between the findings of the proposed model for the buckling analysis of graphene nanoplates and the results from the reference study. This action was undertaken to ensure the accuracy of the system. In the context of this validation, a single-layer nanoplate with a

precise measurement of 201.68 Å in length (illustrated in Figure 2) was carefully analyzed across various aspect ratios. The comparison illustrated in Figure 2 reveals a significant alignment with the reference data, thereby affirming the accuracy and reliability of the developed model.

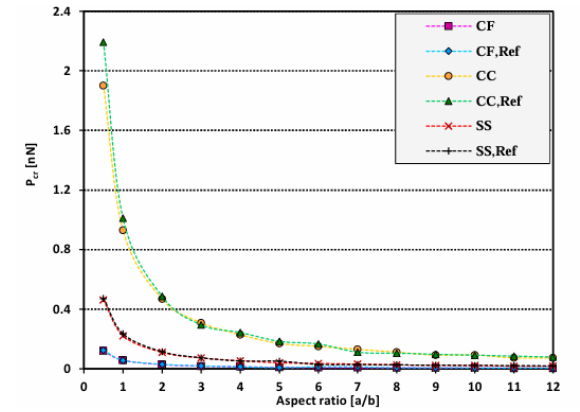

Fig. 2. Comparison and validation of the critical buckling load of a single-layer nanoplate with a length of 201.68 Å

5. RESULTS AND DISCUSSION

This section presents the findings of the buckling analysis conducted on both single-layer and double-layer graphene nanoplates. The study thoughtfully considers whether defects are present or absent. The nanoplates, characterized by widths of 30 Å and 70 Å, along with varying aspect ratios, are examined under three specific boundary conditions: CF, CC, and SS. A uniform compressive force (P) is applied at one end of the plates.

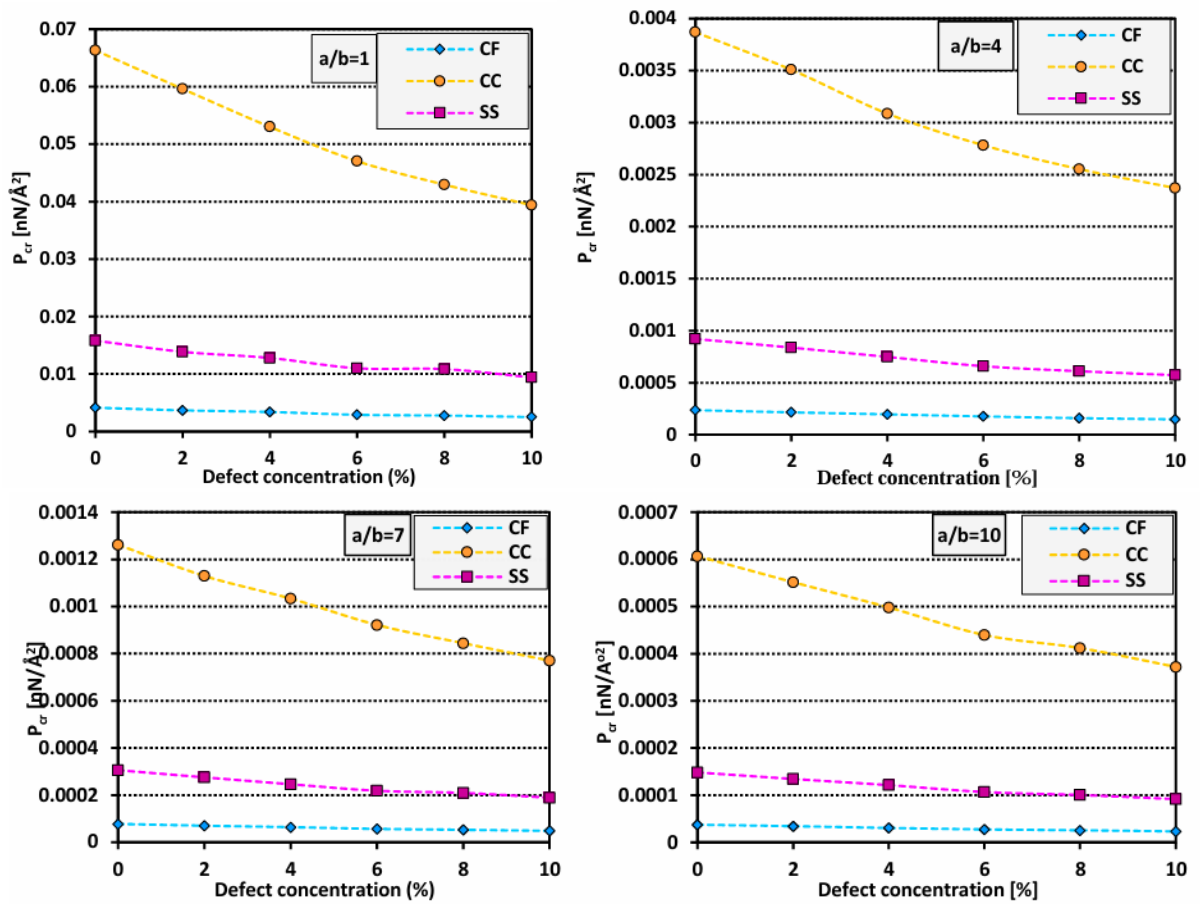

Fig. 3. Effect of defects on *Pcr* of a single-layer nanoplate with the width of 30 Å and aspect ratios *a*/*b*=1,4,7,10.

In order to explore the influence of defects on the buckling behavior of the nanoplate, the vacancies were strategically distributed throughout the graphene geometry in a random manner. In the analysis of each nanoplate subjected to various boundary conditions, three distinct cases of vacancy distribution were carefully evaluated, and the corresponding average values were duly reported. Figure 3 present the effects of atomic vacancy on the buckling capacity for one specific widths of single layer graphene, namely 30 Å, across various aspect ratios and under the three boundary conditions that have been introduced. It has been noted that the existence of defects tends to result in

a decrease in the critical buckling load across all scenarios. It is observed that in all graphs, the buckling capacity tends to decrease with the increase in defects, following an almost linear trend. An analysis of the graphs presented in Figs. 3 reveals that the buckling capacity per unit area of the wider structure, measuring 70 Å, is lower than that of the narrower structure, which measures 30 Å. This observation aligns with what has been noted for defect-free graphene, and a similar rationale can be applied to explain this behavior.

6. CONCLUSION

An investigation into the buckling behavior of single- layer rectangular nanoplates was conducted using three distinct boundary conditions: clamped-free (CF), clamped-clamped (CC), and simply-simple (SS). Furthermore, another study examined the impact of vacancy flaws. The observations and results presented here have been carefully derived from this investigation:

The findings indicate that both the width and length of the nanoplate influence the buckling capacity per unit cross-sectional area. This indicates that the buckling load is reduced for a width of 70 Å compared to that of 30 Å. It is conceivable that this may be associated with the observation that the likelihood of local buckling increases with the expansion of the sheet width, consequently leading to a reduction in the buckling load capacity of the graphene. At lower values of the aspect ratio, it is observed that the buckling load exhibits a considerable reliance on the aspect ratio. Nonetheless, as the aspect ratio increases, the dependence diminishes in importance. This is applicable to all three boundary conditions. The analysis of boundary conditions reveals that the buckling load generated by CC is the most significant, with SS and CF following in succession. It has come to our attention that the influence of the boundary conditions tends to diminish with an increase in the size and aspect ratio of the object. As the domain expands, the proportion of boundary edges relative to the entire domain diminishes, leading to a reduced influence of boundary conditions. This is a crucial aspect to emphasize from a physical perspective.

REFERENCES

[1] H. Tong-Wei, H. Peng-Fei, W. Jian, W. Ai-hui, Molecular dynamics simulation of a single graphene sheet under tension, New Carbon Mater. 25 (2010) 261–266

[2] A. Nassar, E. Nassar, I. Rivilla, J. Labidi, A.G. Fernandez, F. Sarasini, Enhancing the thermal conductivity and shape stability of phase-change composites using diatomite and graphene nanoplates for thermal energy storage, Results Eng. 22 (2014) 102184.

[3] J.-S. Moon, D.K. Gaskill, Graphene: Its fundamentals to future applications, IEEE Trans. Microw. Theory Tech. 59 (2011) 2702–2708.

[4] Y. Xu, Z. Guo, H. Chen, Y. Yuan, J. Lou, X. Lin, H. Gao, H. Chen, B. Yu, In-plane and tunneling pressure sensors based on graphene/hexagonal boron nitride heterostructures, Appl. Phys. Lett. 99 (2011).

[5] G.W. Rogers, J.Z. Liu, Graphene actuators: quantum-mechanical and electrostatic double-layer effects, J. Am. Chem. Soc. 133 (2011) 10858–10863.

[6] M. Ryzhii, A. Satou, V. Ryzhii, T. Otsuji, High-frequency properties of a graphene nanoribbon field-effect transistor, J. Appl. Phys. 104 (2008).

[7] C.-T. Hsieh, B.-H. Yang, J.-Y. Lin, One-and two-dimensional carbon nanomaterials as counter electrodes for dye-sensitized solar cells, Carbon N. Y. 49 (2011) 3092–3097.

[8] L. Yang, L. Zhang, T.J. Webster, Carbon nanostructures for orthopedic medical applications, Nanomedicine. 6 (2011) 1231–1244.

[9] C. Li, T.-W. Chou, A structural mechanics approach for the analysis of carbon nanotubes, Int. J. Solids Struct. 40 (2003) 2487–2499.

[10] L. Wang, Q. Zhang, Elastic behavior of bilayer graphene under in-plane loadings, Curr. Appl. Phys. 12 (2012) 1173–1177.

[11] M.C. Wang, C. Yan, L. Ma, N. Hu, M.W. Chen, Effect of defects on fracture strength of graphene sheets, Comput. Mater. Sci. 54 (2012) 236–239.

[12] S.F. Heydari, M. Shahgholi, A. Karimipour, M. Salehi, S.A. Galehdari, The effects of graphene oxide nanoparticles on the mechanical and thermal properties of polyurethane/polycaprolactone nanocomposites; a molecular dynamics approach, Results Eng. 24 (2014) 102933.

[13] K. Behfar, R. Naghdabadi, Nanoscale vibrational analysis of a multi-layered

graphene sheet embedded in an elastic medium, Compos. Sci. Technol. 65 (2005) 1159–1164.
[14] K. Behfar, P. Seifi, R. Naghdabadi, J. Ghanbari, An analytical approach to determination of bending modulus of a multi-layered graphene sheet, Thin Solid Films. 496 (2006) 475–480.
[15] S. Kitipornchai, X.Q. He, K.M. Liew, Continuum model for the vibration of multilayered graphene sheets, Phys. Rev. B—Condensed Matter Mater. Phys. 72 (2005) 75443.
[16] A. Jafari, S.S. Shah-enayati, A.A. Atai, Size dependency in vibration analysis of nano plates; one problem, different answers, Eur. J. Mech. 59 (2016) 124–139.
[17] S.F.A. Namin, R. Pilafkan, Vibration analysis of defective graphene sheets using nonlocal elasticity theory, Phys. E Low-Dimensional Syst. Nanostructures. 93 (2017) 257–264.
[18] B. Liu, Z. Zhang, Y. Chen, Atomistic Statics Approaches—Molecular Mechanics, Finite Element Method and Continuum Analysis, J. Comput. Theor. Nanosci. 5 (2008) 1891–1913.
[19] A. Alidoust, M. Haghgoo, R. Ansari, J. Jamali, M.K. Hassanzadeh-Aghdam, A numerical conductive network model for investigating the strain-sensing response of graphene nanoplatelets-filled elastomeric strain sensors, Results Eng. 24 (2014) 103341.
[20] B. Liu, Y. Huang, H. Jiang, S. Qu, K.C. Hwang, The atomic-scale finite element method, Comput. Methods Appl. Mech. Eng. 193 (2004) 1849–1864.
[21] B. Liu, H. Jiang, Y. Huang, S. Qu, M.-F. Yu, K.C. Hwang, Atomic-scale finite element method in multiscale computation with applications to carbon nanotubes, Phys. Rev. B—Condensed Matter Mater. Phys. 72 (2005) 35435.
[22] X. Guo, A.Y.T. Leung, X.Q. He, H. Jiang, Y. Huang, Bending buckling of single-walled carbon nanotubes by atomic-scale finite element, Compos. Part B Eng. 39 (2008) 202–208.
[23] S.C. Pradhan, Buckling of single layer graphene sheet based on nonlocal elasticity and higher order shear deformation theory, Phys. Lett. A. 373 (2009) 4182–4188.
[24] A.T. Samaei, S. Abbasion, M. Mirsayar, Buckling analysis of a single-layer graphene sheet embedded in an elastic medium based on nonlocal Mindlin plate theory, Mech. Res. Commun. 38 (2011) 481–485.
[25] Y. Zhang, L.W. Zhang, K.M. Liew, J. Yu, Buckling analysis of graphene sheets embedded in an elastic medium based on the kp-Ritz method and non-local elasticity theory, Eng. Anal. Bound. Elem. 70 (2016) 31–39.
[26] A. Sakhaee-Pour, Elastic buckling of single-layered graphene sheet, Comput. Mater. Sci. 45 (2009) 266–270.