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Variation Percentage In Critical Buckling Load Of Defective Nanoplates Of Single-Layer Graphene As A Function For Different Boundary Conditions

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ABSTRACT

This study examines the bending behavior of single-layer armature-type graphene nanoplates of varied diameters due to variable-distribution atomic vacancy defects. This study is novel because it thoroughly examines the effects of aspect ratio, defect concentration, clamped-free (CF), clamped-clamped (CC), and simply-supported (SS) boundary conditions on graphene nanoplate buckling. Novel space frame structures were employed to characterize nanoplates to preserve their discreteness. The finite element approach anticipated buckling. The simulation results for the critical buckling load (Pcr) were confirmed by comparing them to accessible literature data. Results show that reducing this factor significantly decreases Pcr at low aspect ratios, whereas the loss becomes slow at higher aspect ratios. Research indicates that atomic-scale errors considerably reduce Pcr, with a 10% concentration resulting in a 40% drop in critical buckling stress, highlighting the significance of defects in nanostructure stability.

Keywords: Defective Nanoplates; Critical Buckling Load; Boundary Conditions.

1. INTRODUCTION AND LITERATURE REVIEW

Nanoplates, which have nanoscale structures with two dimensions, have recently attracted a lot of attention from researchers. Numerous studies have focused on graphene sheets, both single-layer and multilayer, due to its remarkable properties and extensive range of potential applications [1,2].

Graphene, the strongest and thinnest material known, has garnered interest because to its outstanding mechanical, electrical, and thermal capabilities. Graphene nanoplates have unique properties that make them a promising material for many applications in many sectors. These include biomedical

technologies, solar energy systems, transistors, electromechanical devices, nanosensors, and nanoactuators. There is a lot of theoretical and experimental research looking at the behavior of these materials under different operating conditions because they could change the electronics, energy storage, and healthcare industries. The first group of theoretical studies use computational methods and the finite element method (FEM) from the perspectives of atomic, continuum, and molecular mechanics. Despite the inherent limitations of each method, a number of researchers have employed them to investigate graphene and other nanostructures in detail. Density functional theory, tight-binding, and molecular dynamics (MD) are atomic-based methods that have reliably and correctly studied the mechanical behavior of single-layer graphene sheets [9]. Using molecular dynamics simulations, several researchers have investigated the mechanical properties of graphene sheets, such as their ultimate strength, Young's modulus, and temperature-dependent changes in these parameters. A recent study by Wang and Zhang used MD simulations to calculate the Young's modulus and fracture toughness of bilayer graphene. The results showed that although temperature had a little impact on the elastic modulus, it significantly affects fracture toughness [10]. Graphene with vacancies and Stone-Wales (S-W) flaws failed to meet expectations, according to a separate study by Wang et al. [11]. Fadaei Heydari et al. [12] used MD simulations to study the effects of graphene oxide nanoparticles (GO-NP) on the thermal and mechanical properties of PU/PCL nanocomposites. They found that a 2% GO-NP concentration was the sweet spot, enhancing mechanical strength, heat flux, and thermal conductivity without sacrificing any of the material's other desirable properties.

Second theoretical method is based on continuum-based technology, which effectively models the small-scale structures' distinctive properties. This technique was used by Behfar and Naghdabadi to investigate the vibration properties of multilayer graphene sheets immersed in an elastic media [13]. An analytical method for predicting the flexural modulus of multilayer graphene sheets was also presented in another paper [14]. A continuum-plate model was constructed by Kitipornchai et al. [15] to evaluate the vibrations of multilayer graphene sheets.

Using both classical and non-classical theories, such as the implicit gradient, non-local differential form, first-order strain gradient, and second-order strain gradient, Jafari et al. [16] examined the free vibration behavior of nanoplates. They studied the influence of parameters including classical and nonlocal features, boundary conditions, and plate dimensions while numerically solving partial differential equations and deriving parametric responses for natural frequencies using the Navier and Galerkin techniques. Also, using nonlocal elasticity theory, Namin and Pilafkan [17] investigated the vibrational behavior of flawed graphene sheets and found that the inherent frequencies of these sheets are reduced due to atomic structural flaws.

The limitations of atomic and continuum-based simulations on scaling have prompted the development of multiscale computing techniques and a third theoretical perspective. These approaches integrate molecular mechanics with finite element methods (FEM) to produce FEM models at the atomic scale that faithfully depict atomic interactions, force fields, and nanoscale phenomena while avoiding the usual FEM approximations. This approach allows for the evaluation of the buckling force, natural frequencies, and vibration modes of carbon nanostructures while reducing computing costs in comparison

to molecular dynamics simulations [18, 19].

The atomic finite element method (AFEM) was initially introduced by Liu et al. [20], and its application was later broadened to study the mechanical properties of carbon nanotubes with a single wall [21]. Using AFEM, Gu et al. [22] examined local buckling in bent single-walled carbon nanotube models by plotting strain energy curves. In a similar vein, Pradhan [23] looked into the effects of nanoscale factors on the critical buckling stress of single-layer graphene and discovered that buckling ratios increased with nonlocal parameter values and decreased with graphene sheet length. Use of nonlocal Mindlin plate theory was employed by Samaei et al. [24] to characterize single-layer graphene sheets and assess their buckling behavior in an elastic medium. The effect of nonlocal factors and the element-free Kp-Ritz technique on critical buckling patterns was studied by Zhang et al. [25] in their study of single-layer graphene sheet buckling in elastic environments. Meanwhile, Sakhaee-Pour [26] examined elastic buckling using molecular structural mechanics and found a nonlinear relationship between buckling force and sheet width, in which aspect ratio had no noticeable effect.

2. FEM SIMULATIONS

A combination of ANSYS and MATLAB is used to conduct the numerical simulations. This was accomplished by first developing the model geometry in MATLAB and then importing the data into ANSYS for solution execution and boundary condition application. On top of that, ANSYS command code is generated by a MATLAB script. Figure 1 shows that the model represents the current coordinate system in addition to a two-dimensional structure with dimensions a and b. The modeling process begins with the definition of points that stand in for carbon atoms. Lines representing covalent bonds are then drawn connecting these spots. A whole two-dimensional lattice is formed by producing and duplicating one unit cell along the $x-$ and $y-$axes to generate the planar structure.

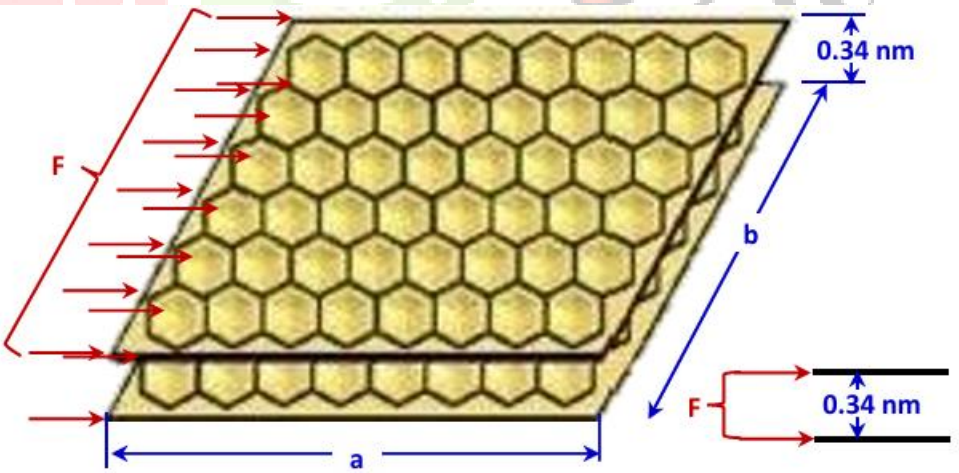

Fig. 1. Interlayer distance in double-layer graphene nanoplates under compression load causing buckling.

To characterize the covalent bonds within the graphene structure, the three-dimensional BEAM4 elastic element was used. This model incorporates three degrees of freedom for translation along the x, y, and z axes and three degrees of freedom for rotation around these axes into every node. We also incorporated interlayer springs to show the van der Waals interactions between the layers next to one other. These interactions were only considered when the distance between atoms was less than or equal to

the cutoff radius, denoted by σ (the Lennard-Jones parameter). It was believed that atoms did not interact with one another at this level. Following their specification across atomic sites, the springs' stiffness values were computed by means of an equivalency approach that linked the springs' elastic energy to the chemical bond energy.

To study the buckling behavior, many nanoplates were tested, each with a distinct length and one of two width values (30 Å or 70 Å). Nanoplates of different lengths were made for each width in order to study the effect of the aspect ratio, a/b. To further illustrate how atomic defects impact the nanoplate's bending capabilities, various vacancy concentrations were introduced to its form. The simulations incorporated the several sorts of boundary conditions described in Table 1 since they also significantly affect buckling behavior. Just to keep things simple, CF stands for clamped-free boundary conditions, CC for clamped-clamped, and SS for simply supported boundary conditions.

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

The results of the reference study and the proposed model for buckling analysis of graphene nanoplates were compared. The system's integrity was ensured by doing this. In order to validate this, several aspect ratios were tested on a perfect single-layer nanoplate that measured 201.68 Å in length (as shown in Figure 2). Figure 2 shows the comparison, which proves the model's accuracy and reliability by showing that there is a lot of agreement with the reference data.

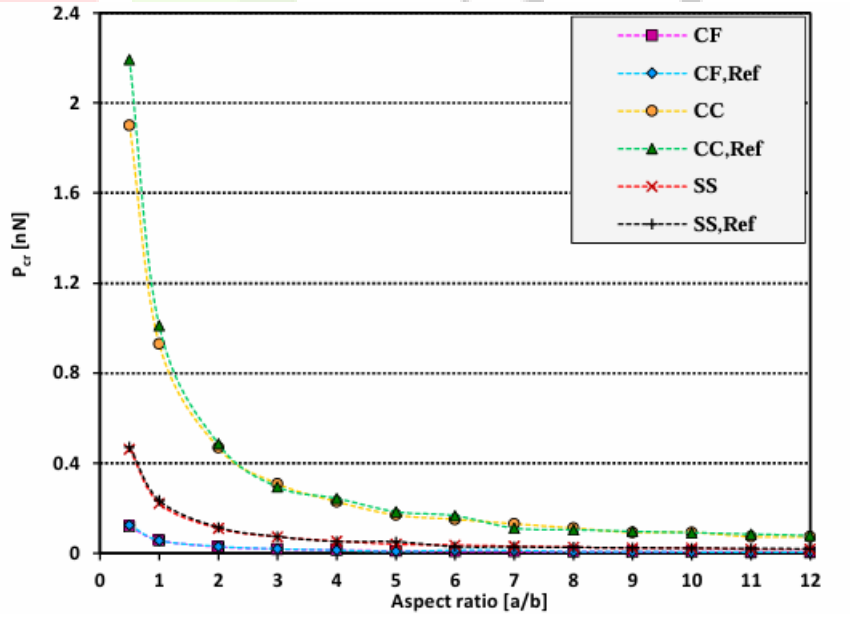

Fig. 2. Comparison and validation of the critical buckling load of a single-layer nanoplate with a length of 201.68 Å

5. RESULTS AND DISCUSSION

Only single-layer graphene nanoplates' buckling analysis findings are given here. The research accounts for the possibility of flaws. A uniform compressive force (***U***) is applied at one end while three separate boundary conditions (CF, CC, and SS) are applied to the nanoplates with widths of 30 Å varying aspect ratios.

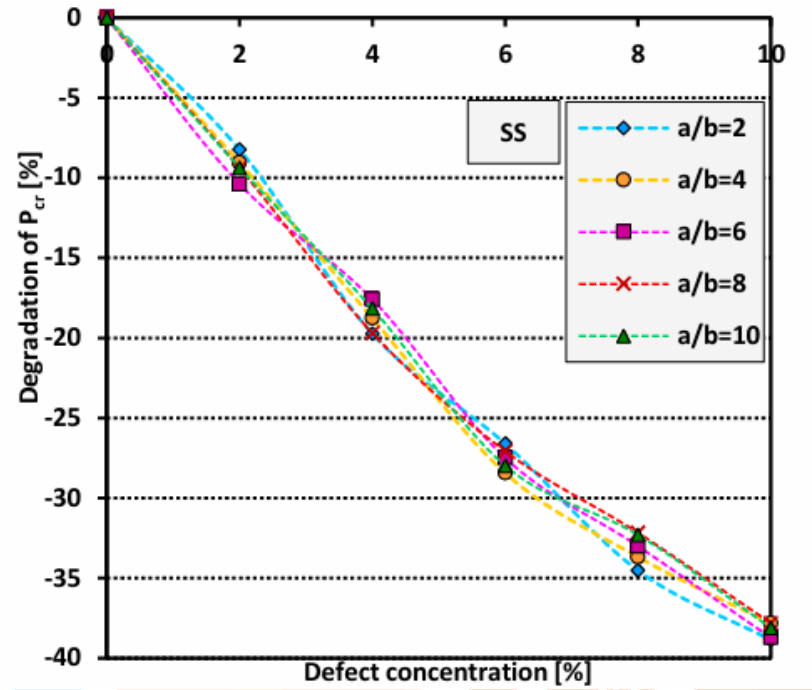

Fig. 3. Variation percentage in *Pcr* of defective nanoplates for 30 Å-width single -layer graphene in SSBC.

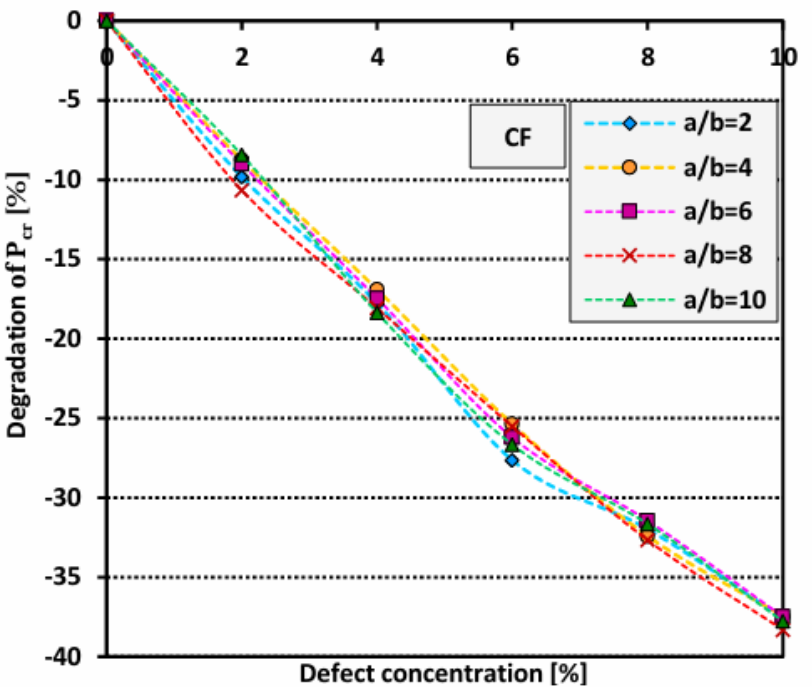

Fig. 4. Variation percentage in *Pcr* of defective nanoplates for 30 Å-width single -layer graphene in CFBC.

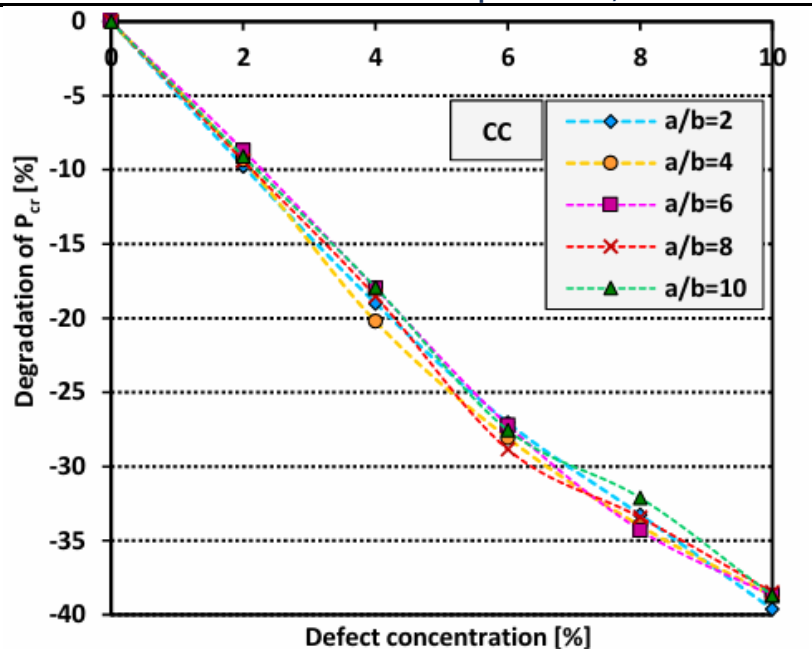

Fig. 5. Variation percentage in *Pcr* of defective nanoplates for 30 Å-width single -layer graphene in CCBC.

In order to give a comparison that is more thorough, the deterioration percentage is defined as the ratio of the buckling load of the faulty graphene to that of the graphene that is free of defects. The findings of this dimensionless factor, expressed as a percentage, are presented in Figures 3 to 5, respectively, in this regard. As an example, a fault concentration of 10% results in a reduction of around 40% in X. As can be seen from these figures, the link between the decrease in defect % and the reduction in defect percentage follows a pattern that is practically linear. Furthermore, the influence of defects on the buckling load is not affected by variations in the aspect ratio, since the curves for various aspect ratios are essentially similar. This is the case regardless of the value of the parameter.

6. CONCLUSION

A study of the buckling behavior of single- and double-layer rectangular nanoplates was conducted using three different boundary conditions: clamped-free (CF), clamped-clamped (CC), and simply-simple (SS). Furthermore, the impact of vacancy faults was explored in another research. This inquiry produced the following findings and results:

Based on the data, it was discovered that the width of the nanoplate, as well as its length, influences the buckling capacity per unit cross section area. The buckling load is smaller at a width of 70 Å compared to 30 Å. This might be due to the fact that the likelihood of local buckling increases as sheet width increases, reducing the graphene's buckling load capacity. At low aspect ratios, the buckling stress is stated to be highly dependent on the aspect ratio. However, when the aspect ratio increases, the dependency becomes less important. This is valid for all three border conditions. In terms of boundary conditions, CC produces the biggest buckling load, followed by SS and CF. It has been observed that the influence of boundary conditions reduces as the size and aspect ratio of the object rise. As the domain's size increases, the proportion of boundary edges relative to the whole domain decreases, reducing the influence of boundary conditions. This is an important issue to note from a physical standpoint.

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