

Buckling Analysis of Graphene Sheets under Nonlocal Effects

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Abstract—The biaxial buckling behavior of single-layered graphene sheets (SLGSs) is studied in the present work. To consider the size-effects in the analysis, Eringen's nonlocal elasticity equations are incorporated into classical plate theory (CLPT). A Generalized Differential Quadrature Method (GDQM) approach is utilized and numerical solutions for the critical buckling loads are obtained. Then, molecular dynamics (MD) simulations are performed for a series of zigzag SLGSs with different side-lengths and with various boundary conditions, the results of which are matched with those obtained by the nonlocal plate model to numerical the appropriate values of nonlocal parameter relevant to each type of boundary conditions.

Keywords—Biaxial buckling, single-layered graphene sheets, nonlocal elasticity, molecular dynamics simulation, classical plate theory.

I. INTRODUCTION

Due to outstanding mechanical, electrical, and chemical properties, the families of carbon nanostructures such as graphene sheets (Fig. 1), carbon nanotubes, and fullerenes provide a new foundation to apply in different emerging fields of nanoscience and nanotechnology [1]–[4]. Because of their small scale, there are some difficulties in conducting experiments to investigate the behaviors of nanostructures which make their theoretical analyses become increasingly important.

Fig. 1 Definition of chiral vector for a graphene sheet

Based on the classical plate theory (CLPT), Kitipornchai et al. [5] investigated the vibration response of multi-layered graphene sheets (MLGSs) with simply-supported boundary conditions using a continuum model. They proposed an explicit formula for the van der Waals interaction between any two sheets of an MLSG. Liew et al. [6] proposed a continuum model to analyze the vibrations of MLSG embedded in an elastic matrix.

As the classical continuum models do not have the capability to consider the size-effects in the analysis of nanostructures, using them to predict the behavior of structures at the nanoscale becomes controversial. Hence, the extension of the continuum mechanics to accommodate the size dependence of

nanostructures is a topic of major concern. Modified continuum models are one of the most applied theoretical approaches for the investigation of nanomechanics due to their computational efficiency and their capability to produce accurate results which are comparable to those of the atomistic models [4]. The application of nonlocal continuum mechanics allowing for the small scale effects in the analysis of nanostructures has been recommended by many research workers.

Ansari et al. [7] developed a nonlocal finite element model to investigate the vibrations of MLGSs with different boundary conditions embedded in an elastic medium. Shen and his assistances [8] studied the nonlinear vibrations of simply supported SLGSs in thermal environment based on nonlocal orthotropic plate model. The vibration analysis of MLGSs embedded in a polymer matrix was investigated by Pradhan and Phadikar [9] using nonlocal continuum mechanics.

Continuing with the nonlocal continuum applications, Murmu and Pradhan [3] developed a single-elastic beam model to analyze the thermal vibration of CNTs based on thermal elasticity mechanics, and nonlocal elasticity theory. nonlocal scale parameter effects on the wave propagation in multi-walled carbon nanotubes was represented by Narendar and Gopalakrishnan [10]. Arash and Ansari [11] studied the vibration characteristics of single-walled carbon nanotubes (SWCNTs) based upon a nonlocal shell model. There are so many other researches in which the behaviors of nanostructures under various loading conditions have been predicted based on continuum elastic models [12], [13], which indicates the wide range of application of this type of modified continuum mechanics in the nanomechanics.

II. NONLOCAL ELASTICITY THEORY

The essence of the nonlocal elasticity theory is that the stress field at a reference point x in an elastic continuum depends not only on strain at that point but also on strains at all other points in the body. This is in accordance with the atomic theory of lattice dynamics and experimental observations on phonon dispersion. The scale effects are accounted for in the theory by considering internal size as a material parameter. The most general form of the constitutive relation for nonlocal elasticity involves an integral over the whole body. According to the nonlocal elasticity theory initiated by Eringen [14], the nonlocal constitutive equation in differential form can be written as:

Fig. 2 Schematic of a biaxially compressed monolayer GS

The bending and twisting moments per unit length are given by:

$$M_x = -D \frac{\partial^2 w}{\partial x^2} - \frac{D}{l^2} \frac{\partial^4 w}{\partial x^4}$$

$$\int_{-a/2}^{a/2} \int_{-a/2}^{a/2} M_{xx} M_{yy} M_{xy} dz \quad (4)$$

With the principle of virtual work, the equilibrium equation governing the buckling of biaxially compressed plates takes the form:

$$D \nabla^4 w - P_x \nabla^2 w - P_y \nabla^2 w = 0 \quad (5)$$

where P is the critical biaxial buckling load. Using (2) and (4), one can arrive at the nonlocal governing equation of (5) in terms of displacements as:

$$D \nabla^4 w - P_x \nabla^2 w - P_y \nabla^2 w - \frac{Eh^3}{12(1-\nu^2)} \nabla^2 w = 0 \quad (6)$$

III. GDQM SOLUTION PROCEDURE

The DQ method has been proved to be an efficient higherorder numerical technique for the solution of initial and boundary value problems. The DQ technique has been widely reported to yield successful solutions for various dynamic and stability problems [15]-[17].

The mth-order derivative of a single function f(x) at a given discrete grid point i can be approximated by the DQ method with N discrete grid points as:

$$\frac{\partial^m f(x_i, y_j)}{\partial x^m} = \sum_{j=1}^N w_{ij}^{(m)} f(x_j, y_j); \quad i=1,2,\dots,N \quad (7)$$

where N is the number of grid points in the x-direction and $w_{ij}^{(m)}$ represents the respective weighting coefficient related to the mth-order derivative. So, for example, if $m = 1$, the first-order derivative is obtained as follows:

$$\frac{\partial f(x_i, y_j)}{\partial x} = \sum_{k=1, k \neq i}^N w_{ik}^{(1)} f(x_k, y_j) \quad (8)$$

where the superscript (m) and (m + 1) denote the order of the derivative. The number of discrete grid points and the grid point distribution can be chosen arbitrarily in the implementation of the

DQM. However, it is shown that the grid point distribution, which is based on well-accepted Gauss–Chebyshev–Lobatto points [18], gives sufficiently accurate results. The coordinates of the grid points are as follows:

$$x_i = a \cos \frac{i\pi}{2N+1}; \quad i=3,4,\dots,N-2; \quad (9)$$

$$x_1 = 0, x_2 = a, x_N = a, x_{N-1} = 0, = 10^{-5}$$

$$y_1 = 0, y_2 = b, y_N = b, y_{N+1} = b, = 1 \dots 10 \dots 05 \quad (10) 2$$

where N is the number of grid points in the y-direction and M is the number of grid points in the x-direction. In the case of the rectangular graphene sheet, the computational domain is $0 \leq x \leq a$ and $0 \leq y \leq b$. In the present case same numbers of grid points are used in x and y directions ($N=M$). As it was previously mentioned, a and b are the length and width of the grapheme sheet, respectively. Here, it is assumed that the thickness of the plate is constant. GDQM can be used to deal with complicated problems reasonably well because its implementation is very simple.

For convenience and generality (6) we introduce the following nondimensional parameters:

$$y_1 = 0, y_2 = b, y_N = b, y_{N+1} = b, = 1 \dots 10 \dots 05$$

$$W = w/a, \bar{y} = y/b, \bar{x} = x/a, N = \frac{a}{D}, \bar{a} = \frac{a}{a}, \bar{b} = \frac{b}{a}, \bar{D} = \frac{D}{a} \quad (11)$$

Substituting (11) into (6), we have the nonlocal governing equation for compressed plate in nondimensional form:

$$D^4 W - PL^2 D^2 W + e a D^2 W - Eh^3 W = 0 \quad (11)$$

$$D^4 W - PL^2 D^2 W + e a D^2 W - Eh^3 W = 0 \quad (12)$$

Transformation of continuous boundary conditions into discretized form under GDQ rule mapping is performed by a direct substitution of these conditions into governing equations, as shown in [18]:

boundary conditions by modified weighting coefficient method [18], we write (12) in the nondimensional form:

$$\sum_{k=2}^{N_x-1} A_{ik(4)kj} W_{ik(4)kj} + \sum_{m=1}^{N_y-1} A_{ik(2)B} W_{jm(2)km} + \sum_{m=1}^{N_y-1} B_{jm(4)} W_{jm(4)} = 0 \quad (16)$$

It should be noted that the (18) is solved for inner grid points. DQ procedures could be advantageous in dealing with nonlocal elasticity problems of small scale structures over other approaches because its implementation is very simple and could handle complicated problems reasonably well. These problems include nonlocal Mindlin plate theory or

is $0 \leq x \leq 1; 0 \leq y \leq 1$. Making use of (7) and incorporating the

higher order nonlocal plate theories with axially stressed reduced to an eigenvalue problem:

$$[K] W = N W_{total} \quad (17)$$

where N^0 is the nondimensional buckling load described in (11). The (17) can be solved by a standard eigenvalue solver conditions. The above DQ analogous (16) can easily be

From this solution the buckling loads of graphene sheets

All edges simply supported (SSSS):

$$W = 0, \sum_{m=1}^{N_y-1} B_{jm(2)lm} W_{jm(2)lm}; i = 1, N_x; \text{ At } x=0, x=a \quad (13)$$

$$W = 0, \sum_{k=1}^{N_x-1} A_{ik(2)kj} W_{ik(2)kj}; j = 1, N_y; \text{ At } y=0, y=b$$

All edges clamped (CCCC):

SSSS	1.86
CCCC	1.17
CCSS	1.52

The variation of obtained critical biaxial buckling loads with the side-length of square SLGSs is illustrated in Figs. 5–7 relevant to different values of nonlocal parameter with different boundary conditions.

Table II presents the appropriate values of μ derived through fitting procedure corresponding to different types of boundary conditions. It is evident that there is an excellent agreement between the results of MD simulations and the ones predicted by the present nonlocal continuum plate model with their appropriate values of nonlocal parameter.

VI. CONCLUSION

Biaxial buckling characteristics of SLGSs were investigated in this work. To this end, Eringen’s nonlocal elasticity equations were incorporated into classical plate theory (CLPT) to consider the size-effects in the biaxial analysis. GDQM form of numerically solution was conducted to obtain the critical biaxial buckling loads of SSSS, CCCC and CCSS square SLGSs with different values of side-length and nonlocal parameter.

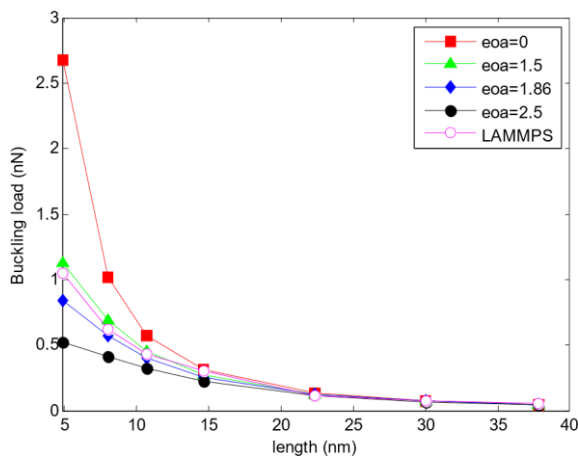


Fig. 5 Variation of critical biaxial buckling load with side-length of square SLGS corresponding to the different values of nonlocal parameter for nonlocal CLPT and comparison with MD simulation for SSSS

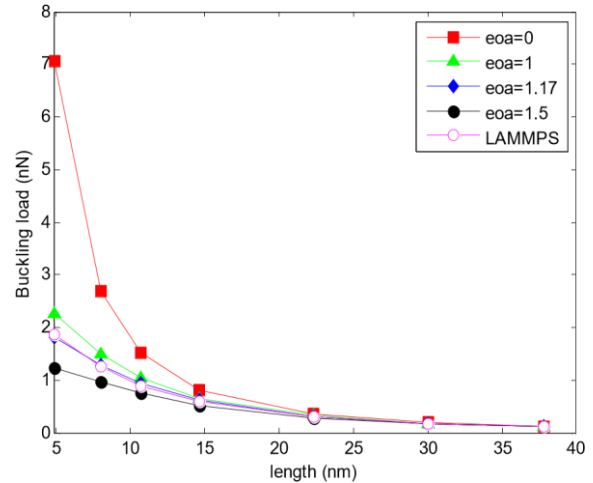


Fig. 6 Variation of critical biaxial buckling load with side-length of square SLGS corresponding to the different values of nonlocal parameter for nonlocal CLPT and comparison with MD simulation for CCCC

Afterward, MD simulations were performed for zigzag SLGSs with different values of side-length, and boundary conditions the results of which were fitted with those calculated by the nonlocal elasticity plate model through a least-square fitting procedure to extract the correct values of nonlocal parameter corresponding to each type of boundary conditions. It was revealed that nonlocal elasticity theory can estimate the biaxial buckling response of SLGSs with great accuracy using the proposed values for the nonlocal parameter, which is comparable to the results of MD simulation. This analysis showed that the importance of the small length scale is dependent on the boundary conditions of SLGS.

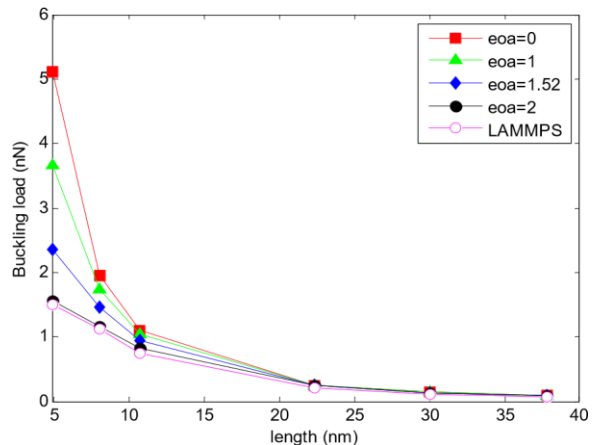


Fig. 7 Variation of critical biaxial buckling load with side-length of square SLGS corresponding to the different values of nonlocal parameter for nonlocal CLPT and comparison with MD simulation for CCSS

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