SMALL SCALE EFFECT ON THE BUCKLING ANALYSIS OF DOUBLE-LAYER GRAPHENE NANORIBBONS EMBEDDED IN AN ELASTIC MATRIX

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1. General Introduction

A Graphene crystal is an infinite two-dimensional layer consisting of sp² hybridized carbon atoms, which has sparked much interest [1]. Graphene nanoribbons (GNRs), belonging to graphene sheets (GSs) and possessing large aspect ratio, have been a hot-spot because of their remarkable electronic [2], thermal [3] and mechanical properties [4, 5]. There are some available methods to produce GNRs. Kosynkin et al. [6] successfully synthesized GNRs by oxidative unzipping of carbon nanotubes (CNTs). Cai et al. [7] devised a simple, bottom-up approach to produce GNRs with different topologies and widths. Sen et al. [8] produced GNRs by tearing GSs from adhesive substrates, and discovered the formation of tapered GNRs.

The outstanding mechanical, electronic transport and spin transport properties of GNRs make them attractive materials for a wide range of device applications [9], such as sensors [10, 11]. Therefore, it is important to study the mechanical properties of GNRs. GSs [12] and graphene nanoplatelet [13] are used to be embedded in elastic matrix, such as in polymer composites, for enhancement of strength of the parent materials. So it is useful to research the mechanical property of embedded GNRs in the same.

In the study of mechanical property of GNRs, buckling behavior becomes an important issue concerning application of GNRs recently [4, 5]. M. Neek-Amal et al. [4, 5] have researched buckling behavior of single-layer GNRs subjected to axial stress by MD simulation, and to our mind the buckling stress of double-layer GNRs (DLGNRs), especially of DLGNRs embedded in an elastic matrix is seldom studied. Moreover, DLGNRs have been proposed as the only semiconductor to produce insulating state and switch-off electrical conduction [14]. As a result, the study of buckling behavior of embedded DLGNRs is important.

Considering of small scale effect, the nonlocal elastic theory, which assumes the stress at a reference point is considered as a function of the strain at every point in the body, can present the more reliable analysis than classical elastic theory and has been widely used in buckling analysis of CNTs [15], GSs [16] and other nano-sized materials [17]. Based on the above, in the present work, an analytical procedure based on the continuum model is used to investigate small scale effect on buckling instability of embedded DLGNRs subject to an axial compressive loading.

2. Theoretical Approach

DLGNRs can be studied as a continuum model [18] which is mostly used in theoretical research. Fig.1 (a) shows the continuum model of DLGNRs with length L and width b in a Cartesian coordinate system, in which x and z are the horizontal and vertical coordinates, respectively. The longitudinal cross-section of a DLGNR embedded in an elastic matrix is shown in Fig. 1 (b) that is used in this study. The thickness of each layer of DLGNRs is defined as h that equals to the diameter of a carbon atom, 0.34 nm. The upper and lower layers of DLGNRs are coupled to each other by the van der Waals (vdW) interaction forces.

2.1 Governing Equations

The Euler-Bernoulli beam model assumes that the cross-section of a DLGNR remains planar during flexion and is perpendicular to the neutral axis.
Based on the nonlocal elasticity theory and Euler-Bernoulli beam model, the governing equation for considering small scale effect on an embedded beam subjected to an axial loading $N$ is derived as [19]

$$E I \frac{d^4 w}{dx^4} + N \frac{d^2 w}{dx^2} + (e_0 a)^2 \left( \frac{d^2 p}{dx^2} - N \frac{d^4 w}{dx^4} \right) = p$$

(1)

where $e_0$ is a constant appropriate to each material and $a$ is an internal characteristic length of C-C bond which is found as 0.142 nm. $x$ is the longitudinal coordinate, $w(x)$ is the flexural deflection of the nanoribbon, $p$ is the distributed transverse pressure acting on the nanoribbon per unit axial length, $E$ and $I$ are the elastic modulus and the moment of inertia of graphene nanoribbon, respectively.

For the upper and lower layers of DLGNRs, Eq. (1) is rewritten as

$$E I \frac{d^4 w_1}{dx^4} + N \frac{d^2 w_1}{dx^2} + (e_0 a)^2 \left( \frac{d^2 p_1}{dx^2} - N \frac{d^4 w_1}{dx^4} \right) = p_1$$

(2)

$$E I \frac{d^4 w_2}{dx^4} + N \frac{d^2 w_2}{dx^2} + (e_0 a)^2 \left( \frac{d^2 p_2}{dx^2} - N \frac{d^4 w_2}{dx^4} \right) = p_2$$

(3)

where the subscripts 1 and 2 denote the quantities associated with the upper and lower layers of a DLGNR, respectively.

The Winkler spring model has been used to analyze the mechanical properties of embedded GSs [20], in which the elastic matrix is described as a Winkler model characterized by the spring. The Winkler foundation modulus relative to the elastic matrix is defined as $k_W$ shown in Fig. 1 (b). Then the distributed transverse pressure acting on the upper and lower layers of a DLGNR can be given by

$$p_1 = c (w_1 - w_2) + k_W w_1$$

(4)

$$p_2 = c (w_2 - w_1) + k_W w_2$$

(5)

where $c$ is the vdW interaction coefficient between the upper and lower layers, which can be obtained from the Lennard-Jones pair potential [20, 21], given as

$$c = -b \left( \frac{4 \sqrt{3}}{9a} \right)^2 \frac{24 \zeta}{\delta^2} \frac{\delta}{a} \left[ \frac{3003\pi}{256} \sum_{k=0}^{5} \left( \frac{-1}{2k + 1} \right) \sum_{k=0}^{8} \frac{1}{2k + 1} \right] \left( \frac{\delta}{a} \right)^6 \frac{1}{(\bar{z}_1 - \bar{z}_2)^{12}} - \frac{35\alpha}{8} \sum_{k=0}^{2} \frac{(-1)^k}{2k + 1} \left( \frac{1}{(\bar{z}_1 - \bar{z}_2)^6} \right)$$

(6)

where $\zeta = 2.968$ meV and $\delta = 3.407$ Å are parameters chosen to fit the physical properties of the GNRs. $\bar{z}_i = z_i / a$ ($i = 1, 2$), where $z_i$ is the coordinate of the $i$th layer in the thickness direction with the origin at the mid-plane of the GNRs.

To derive the critical buckling stress in in-phase and anti-phase modes, we assume

$$\xi = w_1 + w_2$$

(7)

$$\eta = w_1 - w_2$$

(8)

Then from the Eqs. (2) and (3), the governing equations of in-phase and anti-phase modes are derived as

$$H_1 \frac{d^4 \xi}{dx^4} + H_2 \frac{d^2 \xi}{dx^2} - k_W \xi = 0$$

(9)

$$H_1 \frac{d^4 \eta}{dx^4} + [H_2 + 2(e_0 a)^2 c] \frac{d^2 \eta}{dx^2} = (2c + k_W) \eta$$

(10)

where

$$H_1 = EI - (e_0 a)^2 \frac{N}{2}$$

(11)

$$H_2 = \frac{N}{2} + (e_0 a)^2 k_W$$

(12)

### 2.2 Boundary Conditions

Consider that a simply supported DLGNR subjected to axial loading $N$ with length of $L$, the corresponding boundary conditions are given as,

$$w_1 = W_1 \sin \left( \frac{m \pi x}{L} \right) \quad m = 1, 2, 3, \ldots$$

(13)

$$w_2 = W_2 \sin \left( \frac{m \pi x}{L} \right) \quad m = 1, 2, 3, \ldots$$

(14)

where $W_1$ and $W_2$ are the amplitudes of displacement in the upper and lower layers of DLGNRs, and $m$ is a positive integer which is related to buckling modes.

Substitute Eqs. (13) and (14) into Eqs. (7) and (8), we obtain

$$\xi = A \sin \left( \frac{m \pi x}{L} \right) \quad m = 1, 2, 3, \ldots$$

(15)

$$\eta = B \sin \left( \frac{m \pi x}{L} \right) \quad m = 1, 2, 3, \ldots$$

(16)

where $A$ and $B$ are the amplitudes of displacement in the in-phase and anti-phase buckling modes of DLGNRs.

### 2.3 Critical Buckling Stress of DLGNRs

Substituting the deflection functions of the DLGNR ($\xi$ and $\eta$) into Eqs. (9) and (10), the critical buckling stress of embedded DLGNRs in in-phase and anti-phase are derived as follows

$$\sigma_{in} = \frac{EI m^4 \pi^4 - (e_0 a)^2 m^2 \pi^2 k_W L^2 - k_W L^4}{b h m^2 \pi^2 (e_0 a)^2 m^2 \pi^2 + L^2}$$

(17)
because

\[
\sigma_{\text{anti}} = \sigma_{\text{in}} = \frac{2(e_0a)^2m^2\pi^2cL^2 + 2cL^4}{h\pi^2[(e_0a)^2m^2\pi^2 + L^2]}
\]  

(18)

3. Results and Discussion

To calculate the critical buckling stress of embedded DLGNRs subject to an axial compressive loading, each layer is modeled as an individual classical thin beam with the same length, width and thickness. The effective thickness of each layer of a DLGNR is equal to the diameter of a carbon atom, 0.34 nm. The aspect ratio of a DLGNR \( L/b \) is larger than 5 because the Euler beam theory produces errors for structures with a small aspect ratio. The Young’s modulus \( E \) and mass density \( \rho \) of the DLGNRs are the same as those of a GS, 1.02 TPa and 2250 kg/m³, respectively [21].

Fig. 2 shows the relationship between the critical buckling stress and buckling modes of un-embedded DLGNRs with different aspect ratio when \( e_0a = 0 \) nm, where Figs. (a) and (b) express critical buckling stress with in-phase buckling modes and anti-phase buckling modes, respectively. In Fig. 2 (a), the critical buckling stresses of DLGNRs with different aspect ratio are all increasing when the in-phase buckling modes increase, which is the same as single-walled CNTs without considering the vdW [22]. On the contrary, as shown in Fig. 2 (b), the critical buckling stresses are all decreasing as the anti-phase buckling modes growing up and the critical buckling stresses of anti-phase buckling mode 1 have the highest values in Fig. 2 (b). Furthermore, as the anti-phase mode increasing to infinity, the buckling stress decreases till to a limit that is still higher than the buckling stress in the first in-phase buckling mode. This is a highlight discovered in the study and has been predicted in our previous work [19]. The explanation is because of the vdW interaction forces between the upper and lower layers of DLGNRs.

The small scale effect on the critical buckling stress of DLGNRs in different in-phase buckling modes is expressed in Fig. 3. We choose aspect ratio \( L/b = 10 \) as a representation for elaborating the local \( (e_0a = 0 \) nm) and nonlocal \( (e_0a = 1.0 \) nm and \( 2.0 \) nm) influence in the critical buckling stress of DLGNRs under an axial compressive loading. It is clearly seen that the critical buckling stresses decrease when \( e_0a \) is from 0 nm to 2.0 nm in all of the in-phase buckling modes. Therefore, the small scale effect makes a negative influence to the critical buckling stress is known, and it is more prominent in higher buckling modes of in-phase buckling modes. Particularly, the critical buckling stresses of DLGNRs in both local and nonlocal influence are nearly the same value in in-phase buckling mode 1.

The small scale effect on the critical buckling stress with the growing aspect ratio is also discussed in this study. The relationship between the aspect ratio of DLGNRs and critical buckling stresses in in-phase buckling mode 1 is shown in Fig. 4. The same as Fig. 3, the small scale effect makes a negative influence to the critical buckling stress. As the aspect ratio of DLGNRs is increasing, the small scale effect becomes less and less till to be ignored, which is agree with small scale effect on the buckling of CNTs well [15].

The Effect of Winkler modulus parameter on the critical buckling stress of embedded DLGNRs with \( e_0a = 0 \) nm and \( L/b = 10 \) is shown in Fig. 5, where Figs. (a) and (b) express critical buckling stress with in-phase buckling modes and anti-phase buckling modes, respectively. The influences of the surrounding elastic matrix on the critical buckling stress are investigated based on the Winkler spring model, and we take the ratio of the Winkler spring modulus to the vdW coefficient \( (k_0/c) \) as a parameter to consider the variation with the stiffness of the elastic matrix. It can be found that for both in-phase and anti-phase buckling modes 1-4, all of the critical buckling stresses of DLGNRs become higher when parameter \( k_0/c \) becomes larger, which means elastic matrix has a positive effect on the critical buckling stress. Furthermore, there is an interesting phenomenon occurs in Fig. 5 (a), the tendency of critical buckling stress curves relating to in-phase buckling mode change from ascent to decline when \( k_0/c \) increases from 0 to 0.1 and 1. The explanation of this phenomenon is the same as the explanation of higher anti-phase buckling mode owns smaller value that is shown in Fig. 2 (b), because we consider the elastic matrix as Winkler spring mode and the critical buckling stresses in anti-phase buckling mode in Fig. 2 (b) are affected by the vdW interaction forces between the upper and lower layers of the DLGNRs which is also treated as spring mode. We also can comprehend this phenomenon by considering the last two terms in the
numerator in Eq. (17), when we substitute $0.1c$ or $c$ to $k_W$.

4. Conclusions

An analytical procedure based on a continuum model is used to investigate small scale effect on buckling instability of DLGNRs embedded in an elastic matrix. The buckling modes of DLGNRs are found to have in-phase and anti-phase modes, in which the deflections of the upper and lower layers occur in the same and opposite directions, respectively. We find that as the buckling modes growing up, the critical buckling stress in anti-phase buckling modes increase whereas the critical buckling stress decrease because of the influence of vdW interaction forces. The small scale effect on the critical buckling stress is also discussed in this study. The results show that the small scale effect makes a negative influence to the critical buckling stress, and the small scale effect becomes less and less when the aspect ratio of DLGNRs is increasing. Furthermore, elastic matrix is described as a Winkler model characterized by the spring and makes a positive effect to the critical buckling stress. In special, the tendency of critical buckling stress curve changes in in-phase buckling modes as the Winkler spring modulus increasing.

Fig. 1 Analytical model. (a) Continuum model of a DLGNR, (b) Longitudinal cross-section of a DLGNR embedded in an elastic matrix.

Fig. 2 Relationship between the critical buckling stress and buckling modes of un-embedded DLGNRs with different aspect ratio. (a) In-phase buckling modes and (b) Anti-phase buckling modes.

Fig. 3 Small scale effect on the critical buckling stress of DLGNRs in in-phase buckling modes.
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Fig. 4 Small scale effect on the critical buckling stress of DLGNRs with different aspect ratio.

Fig. 5 Effect of Winkler modulus parameter on the critical buckling stress of embedded DLGNRs. (a) In-phase buckling modes and (b) Anti-phase buckling modes.

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References


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