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Buckling analysis of pristine and defected graphene

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ABSTRACT

The buckling behavior of monolayer graphene (pristine and vacancy-defected) and bilayer graphene (pristine) loaded in the armchair direction was simulated for different boundary conditions using a truss FE model, representing the exact atomic lattice of graphene, and a FE model of an equivalent 2D plate. The critical buckling stress of pristine monolayer graphene was derived as a function of aspect ratio. The results from the two FE models coincide and are in very good agreement with established analytical solutions. With increasing the aspect ratio, the critical buckling stress of monolayer graphene decreases until the value of 2 from which the effect starts to diminish. Using the truss FE model, the effect of randomly dispersed vacancies on the critical buckling stress and buckling mode of monolayer graphene was studied. It was found that the critical buckling stress decreases dramatically with increasing the defect density: for a defect density of 10%, the critical buckling stress decreases by almost 50%. Moreover, the presence of defects was found to affect the highest buckling modes (above 3) even at low densities. Bilayer graphene has a totally different critical buckling stress than monolayer graphene due to the effect of van der Waals forces which depends on the applied boundary conditions.

1. Introduction

Graphene is an atomic-scale honeycomb lattice composed of carbon atoms. Although it is considered to be the parent material of carbon nanotube, which is probably the most famous material of the 21st century, only recently it has been obtained in a stable crystalline form by Geim and Novolesov [1]. Graphene is not only the thinnest material ever but also the strongest. In [2] Lee et al. have measured, by nanoidentation in an atomic force microscope, the Young's modulus and intrinsic strength of *defect-free* graphene monolayer to be 1.0 TPa and 130 GPa, respectively. In the past, similar values have been also reported for carbon nanotubes but only by simulations. Contrary to simulations, experiments give a Young's modulus of 0.45 TPa and a strength of 40 GPa for carbon nanotubes. The large deviation between simulations and experiments has been found to be attributed to the presence of defects in the nanotube structure [3–6]. Equally significant is the effect of defects on the mechanical properties of graphene. Tserpes [7] has found by atomistic FE simulations that the presence of 4.4% of vacancies (missing atoms) results in a 50% reduction in Young's modulus and tensile strength of graphene.

Among the several potential applications of graphene there are some, such as nano-electromechanical systems, flexible electronics and composite materials that are related with its compressive (buckling) response. Thus, it is important to fully understand the buckling response first of the isolated graphene and then of the embedded graphene. There are a few reported works on the buckling behavior of isolated graphene. Sakhaee-Pour [8] and Rouhi and Ansari [9] used the atomistic FE modeling approach proposed in [10] to derive the elastic buckling force for different boundary conditions and aspect ratios of pristine monolayer graphene. A similar study using a similar method was performed by Chandra et al. [11]. Pradhan [12] derived the same results using nonlocal elasticity and higher order shear deformation theory. Farajpour et al. [13] studied the buckling behavior of nanoscale circular plates under uniform radial compression using a nonlocal continuum plate model. Ansari and co-workers predicted the biaxial buckling and vibration behavior of graphene via a nonlocal atomistic-based plate theory [14] and the biaxial buckling behavior of single-layered graphene sheets based on nonlocal plate models and molecular dynamics simulations [15].

Summarizing this short literature overview it becomes evident that there is still a need for studying the effect of defects on the buckling behavior of graphene and simulating the buckling behavior of multi-layered graphene which is the usual form of graphene. Such a modeling study could be performed either by pure atomistic approaches such as molecular mechanics and dynamics [15] or atomistic-based numerical approaches such as the combination of force-fields with the finite element method [8–10], the nondissipative model based on Hertzian interaction of [16], the universal

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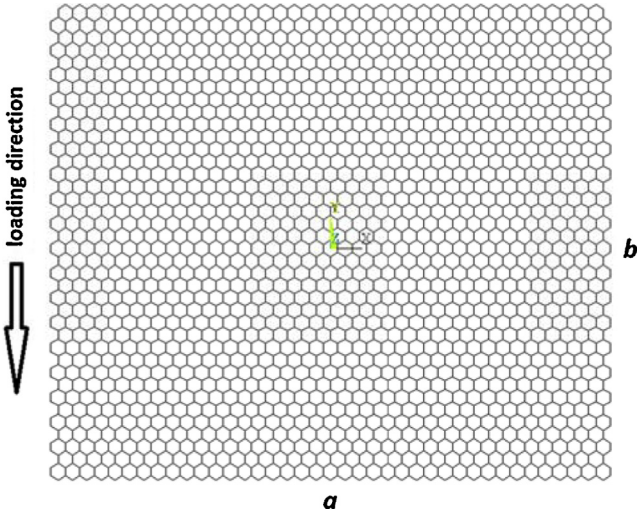

Fig. 1. Schematic of a monolayer graphene, basic dimensions and loading direction.

formulae of [17] and the multi-scale mass-spring models of [17,18]. Both approaches present advantages and disadvantages. The major advantages of atomistic approaches is the accurate representation of atomic structure (geometry of bonds) and the ability to consider chemical phenomena such as bond breaking and formation while their major disadvantages is the large required computational effort and the inability to model systems that lie at scales higher than the nano-scale. On the other hand, the major drawback of atomistic-based numerical approaches is that in some cases they are rather approximate as they fail to model the exact atomic structure and capture chemical phenomena that influence the behavior of the nanomaterial while their major advantage is that they are computationally efficient in the sense they require a very small computational effort and can be used to model complicated material systems lying at different scales and subjected to complex loading conditions. Under this frame, in the present paper, the buckling behavior of monolayer graphene (pristine and vacancy-defected) and bi-layer graphene (pristine) was simulated for different boundary conditions using a truss FE model, representing the exact atomic lattice of graphene, and a FE model of an equivalent 2D plate.

2. Description of problem

Consider a monolayer graphene of height a and width b and a bilayer graphene consisting of two monolayer graphenes. It is desired to compute the critical buckling stress and buckling modes of both pristine materials loaded in the armchair direction for different boundary conditions. In Fig. 1, a schematic of monolayer graphene along with the dimensions and loading direction are illustrated. The boundary conditions considered are listed in Table 1. For graphene monolayer, the effects of aspect ratio (b/a) and randomly dispersed vacancies (1 missing atom) on the critical buckling stress and buckling mode will be also examined. The graphene aspect ratio varied between the values of 0.3 and 2.0.

3. Finite element analysis

To deal with the problem described previously, two different FE models have been developed, namely a truss FE model representing the exact atomic lattice of graphene and a 2D FE model of an equivalent plate. Both models have been developed using the ANSYS FE commercial code [20].

3.1. Truss FE model

Carbon atoms in graphene are bonded together with covalent bonds forming a hexagonal 2D lattice. These bonds have a characteristic bond length and bond angle. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of graphene is the result of the interactions between the bonds. By considering the bonds as connecting load-carrying elements, and atoms as joints of the connecting elements, graphene may be simulated as a plane-frame structure. By treating graphene as a plane-frame structure, its mechanical behavior can be analyzed using classical structural mechanics methods such as the FE method. For the modeling of the C—C bonds, the 3-D elastic BEAM188 element [20] was used. This is a 3D beam element with six DOFs per node. Fig. 2 depicts how the hexagon, which is the constitutional element of graphene nano-structure, is modeled as structural element of a planar-frame. In the same way the entire graphene's lattice is modeled. The modeling simulation leads to the correspondence of the bond length to the element length as well as the wall thickness with the element thickness. By assuming a circular solid cross-sectional area for the element, as in Fig. 2, wall thickness corresponds to element's diameter.

The elastic geometrical properties of the beam elements have been derived using an energy linkage between molecular mechanics and continuum mechanics developed in [10]. According to the linkage the diameter, Young's modulus and shear modulus of the beam elements representing the C—C bonds are derived from:

$$d = 4\sqrt{\frac{k_\theta}{k_r}} \tag{1}$$

$$E = \frac{{k_r}^2 L}{4\pi k_\theta} \tag{2}$$

$$G = \frac{{k_r}^2 k_\tau L}{8\pi {k_\theta}^2} \tag{3}$$

Table 1
Description of the different sets of boundary conditions considered.

Set	$x = a/2$	$x = -a/2$	$y = b/2$	$x = -b/2$
A	– (free)	– (free)	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = -1$	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = 1$
B	– (free)	– (free)	$w = 0$, $\frac{\partial w}{\partial y} = 0$ (clamped) $F_y = -1$	$w = 0$, $\frac{\partial w}{\partial y} = 0$ (clamped) $F_y = 1$
C	$w = 0$, $\frac{\partial^2 w}{\partial x^2} = 0$ (pinned)	$w = 0$, $\frac{\partial^2 w}{\partial x^2} = 0$ (pinned)	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = -1$	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = 1$
D	$w = 0$, $\frac{\partial w}{\partial x} = 0$ (pinned)	$w = 0$, $\frac{\partial w}{\partial x} = 0$ (pinned)	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (clamped) $F_y = -1$	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (clamped) $F_y = 1$
E	$w = 0$, $\frac{\partial^2 w}{\partial x^2} = 0$ (pinned) $F_x = -1$	$w = 0$, $\frac{\partial^2 w}{\partial x^2} = 0$ (pinned) $F_x = 1$	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = -1$	$w = 0$, $\frac{\partial^2 w}{\partial y^2} = 0$ (pinned) $F_y = 1$