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On the buckling of hexagonal boron nitride nanoribbons via structural mechanics

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ABSTRACT

Monolayer hexagonal boron nitride nanoribbons have similar crystal structure as graphene nanoribbons, have excellent mechanical, thermal insulating and dielectric properties and additionally present chemical stability. These allotropes of boron nitride can be used in novel applications, in which graphene is not compatible, to achieve remarkable performance. The purpose of the present work is to provide theoretical estimations regarding the buckling response of hexagonal boron nitride monolayer under compressive axial loadings. For this reason, a structural mechanics method is formulated which employs the exact equilibrium atomistic structure of the specific two-dimensional nanomaterial. In order to represent the interatomic interactions appearing between boron and nitrogen atoms, the Dreiding potential model is adopted which is realized by the use of three-dimensional, two-noded, spring-like finite elements of appropriate stiffness matrices. The critical compressive loads that cause the buckling of hexagonal boron nitride nanoribbons are computed with respect to their size and chirality while some indicative buckled shapes of them are illustrated. Important conclusions arise regarding the effect of the size and chirality on the structural stability of the hexagonal boron nitride monolayers. An analytical buckling formula, which provides good fitting of the numerical outcome, is proposed.

1. Introduction

The hexagonal boron nitride (h-BN) monolayer is analogous to graphene regarding its molecular structure which is made by covalently bonded boron and nitrogen atoms, positioned in a hexagonal manner [1]. Moreover, is a wide bandgap semiconductor and has an excellent thermal as well as chemical stability. Thus, boron nitride nanosheets may be used in devices that work under extreme conditions. Recently, it has been proved that the use of hexagonal boron-nitride multilayer sheets in silica may lead to high performance coatings and electronic devices [2]. These nanosheets are also valued for use in biomaterials, medical, biomedical applications such as drug delivery and in neutron capture therapy [3].

Last decade, the synthesis, structural characteristics and properties of h-BN sheets have significantly drawn the research attention [1]. The main advantage which makes them unique, is that they demonstrate a high thermal and chemical stability [4]. One-atom thick h-BN nanosheets have already been isolated [5] and experimentally investigated via transmission electron microscopy (TEM) [6] and atomic force microscopy (AFM) [7]. Due to the many perspectives of these nanomaterials, many attempts have been made to characterize their mechanical performance, which are based on density functional theory

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(DFT) [8–12], molecular dynamics (MD) [13,14], continuum mechanics (CM) [15,16], structural mechanics (SM) [17–19] and experiments [20].

The design at nanoscale pre-requires not only the knowledge of the elastic and fracture properties of the involved nanomaterials, but also the conditions under which their structural stability is assured. The buckling of the nanomaterials is of high importance especially when compressive stresses are involved. These stresses, even if they are less than the ultimate compressive stress, may cause a failure which is characterized by sudden and unstable deformations. However, few studies about the buckling of boron nitride nanomaterials may be found in the literature and, still, the overwhelming majority of them are associated with boron nitride nanotubes (BNNTs) and grounded on a theoretical basis only. Characteristically, Shokuhfar et al. [21] have investigated the effect of temperature on the compressive buckling of BNNTs by performing MD simulations. Using MD simulations as well, Ebrahimi-Nejad et al. [22] have examined the buckling of perfect and defective armchair BNNTs with different types of vacancy defects. In another attempt, Ebrahimi-Nejad and Shokuhfar [23] have explored the effect of hydrogen physisorption on the compressive buckling strength of BNNTs using MD simulations. The buckling behavior of BNNTs under the action of torsional loadings has been investigated by Ajori and Ansari [24] through the MD method as well. Very recently, Chandra et al. [25] have studied the thermal buckling behavior of precompressed BNNTs using MD simulations and have computed corresponding critical buckling strains. Regarding h-BN monolayer, Sarvi et al. [26] have made an interesting attempt to describe, via explicit expressions obtained by a beam based SM method, the effects of the presence of vacancy defects in a h-BN nanosheet on the buckling loads. In addition, Mohammadimehr and Mohandes [27] have used classical plate theory to study the effect of size on the buckling of a functionally graded double-layer boron nitride plate under electro-thermo-mechanical loadings.

In the present study, the buckling behaviour of various h-BN nanoribbons (h-BNNRs) is investigated by using a structural mechanics (SM), finite element method which utilizes appropriate three-dimensional (3d), spring-like, finite elements to simulate the interatomic force field observed between atoms. The proposed numerical formulation, which is an extension of a previously presented method [28], permits simple modelling and requires a low computational effort in contrast with other standard atomistic simulation tools such as MD. The adopted field is based on the Dreiding model [17] which effectively describes the bond length, interbond angle and dihedral angle changes within the h-BN nanosheets. To the author's best knowledge, it is the first time that the critical compressive loads at which the h-BNNRs become elastically unstable, are numerically predicted by this SM approach. The influence of the size and chirality of the h-BN nanosheets on their critical buckling load is thoroughly investigated. The impact of the boundary conditions on the buckling of the h-BNNRs under compression is also discussed. Finally a predictive analytical buckling formula is proposed.

2. Potential energy

For single walled nanostructures, the van der Waals forces may be neglected. This is a common numerical strategy since van der Waals forces have insignificant effect on the mechanical behavior of monolayer graphene-like nanomaterials. Typically, such kind of forces are simply simulated via the use of appropriate non-linear spring elements when multi-layered molecular structures are to be investigated. Furthermore, by considering small strains, their total potential energy U_{tot} may be expressed as a sum of energies produced due to bond length, interbond angle and dihedral angle changes [29]:

$$U_{\text{tot}} = \sum U_r + \sum U_\theta + \sum U_\tau \tag{1}$$

where the potential energies U_r, U_θ, and U_τ correspond to the two-body (2b), three-body (3b), and four-body (4b) interatomic interactions and are given, respectively, by:

$$U_r = \frac{1}{2}k_r(\Delta r)^2 \tag{2}$$

$$U_\theta = \frac{1}{2}k_\theta(\Delta\theta)^2 \tag{3}$$

$$U_\varphi = \frac{1}{2}k_\tau(\Delta\varphi)^2 \tag{4}$$

where Δr, $\Delta\theta$, and $\Delta\varphi$ represent the bond length, interbond angle, and dihedral angle changes, respectively while k_r, k_θ, and k_φ are the corresponding stiffness constants.

According to the Dreiding model for h-BN nanostructures [17] the stiffness constants k_r, k_θ, and k_φ are equal to 486.5 $nN\ nm^{-1}$, 0.6952 $nN\ nm\ rad^{-2}$, and 0.6255 $n\ N\ nm\ rad^{-2}$, respectively.

The force field appearing within the h-BN nanostructure, may be derived by differentiating Eqs. (2)–(4), evidently leading to linear force-displacement and moment-angle variations. Since problems of linear elastic buckling are investigated here, the linear approximation of the force field is considered adequate.