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An improved molecular structure mechanics method and its application for graphene wrinkling

C.G. Wang[a,b,*], Z.M. Xia[a], H.F. Tan[a]

[a] Center for Composite Materials, Harbin Institute of Technology, Harbin 150001, PR China
[b] National Key Laboratory of Science and Technology on Advanced Composites in Special Environments, Harbin Institute of Technology, Harbin 150080, PR China

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ABSTRACT

This paper proposes an improved molecular structure mechanics (iMSM) method to study the wrinkling characteristics of annular graphene sheet (AGS). An idea of variable cross-section beam, combined with 3-node Timoshenko beam, is introduced in the iMSM model for considering the flexibility of C-C bond and C-C joint simultaneously, and the stiffness matrix of beam element is deduced for later calculation. The parameters of equivalent beam are obtained by using an interior point optimization approach. Based on the proposed iMSM model, the wrinkling characteristics of AGS are simulated, which are verified by molecular dynamic (MD) simulation. A predicted model is used to evaluate the wrinkling level of AGS, which agrees well with the iMSM simulation, and then the effects of beam parameters on graphene wrinkling are also analyzed. The results indicate that our proposed model is reliable to the wrinkling analysis of AGS and may be further used for other researches on graphene.

1. Introduction

Graphene sheet (GS) presents superior mechanical and physical performance such as high Young's modulus and unique electrical property, which has been extensively used for various nanosized resonators and sensors (Lee, Wei, Kysar, & Hone, 2008; Garcia-Sanchez et al., 2008; Geim, 2009). Such amazing physical properties, including vibration, electricity, and magnetic field, have close connection with the configuration of GS. Featuring a planar geometry only one atom thick, GS is apt to generate the out-of-plane deformation spontaneously under different situations, such as mechanical loadings, defects, ripples, chemical functional groups, which will induce wrinkles in GS inevitably, and wrinkles will further intensify the deformation. Therefore, in order to better utilize these properties and design new nanodevices, it is necessary to make the study of wrinkling behavior of GS.

Currently different methodologies have been developed for physical properties of GS, mainly including molecular dynamic (MD), continuum theory model (CTM), and molecular structure mechanics (MSM). Compared with the studies based on MD (Inui, Mochiji, & Moritani, 2008; Herrero & Ramírez, 2009; Wang, Liu, Lan & Tan, 2013) and CTM (Wang, Mylvaganam & Zhang, 2009; Bathe, Chapelle & Lee, 2003; Gil, Adhikari, Scarpa & Bonet, 2010; Wang, Lan, & Tan, 2013; Naderi & Saidi, 2014; Sfyris, Sfyris, & Galiotis, 2014), the study based on MSM can consider the features of atomistic scale structure but is not perplexed in time scales.

* Corresponding author.
E-mail address: wangcg@hit.edu.cn (C.G. Wang).

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With regard to MSM, it has been widely used for the studies of GS property, pioneered by Odegard, Gates, Nicholson and Wise (2002) and Li and Chou (2003). Fundamental to this method is notion that beam members are used with appropriate mechanical parameters to simulate C-C bonds by establishing a linkage between structure mechanics and molecular mechanics. At present, considering the flexibility of C-C bonds, there are various types of beam element and beam cross-section selected. Tserpes and Papanikos (2005) used classical MSM method and assumed a circular cross-section Euler beam to investigate the effect of wall thickness, diameter and chirality on the elastic moduli of single-walled carbon nanotubes (SWNTs). Pour, Ahmadian and Naghdabadi (2008) used the above method to study the vibrational characteristics of GS and the influences of chirality and boundary conditions on natural frequencies were investigated. To capture the distinguishing in-plane σ-σ and out-of-plane σ-π bond angle bending rigidities of C-C bonds, Li and Guo (2008) proposed a rectangular cross-section Euler beam to calculate the elastic moduli of SWNTs. An important contribution of this model is that the five independent elastic moduli of SWNTs can be evaluated systematically. Shakouri, Ng and Lin (2011) presented an elliptical cross-section beam model for the difference between in-plane bending stiffness and out-of-plane bending stiffness. Based on this model, Zhang, Duan, and Wang (2013) proposed a novel model that the cross-section of beam is elliptical but eccentric and used this model to predict wrinkles in annular graphene under circular shearing. The wave numbers, as well as amplitudes and wavelengths are in good agreement with MM results. Considering that the beam thickness is equal to 0.147 nm and the length is 0.142 nm by Tserpes and Papanikos (2005), the beam belongs to the category of deep beam. Therefore it is necessary to take the shear deformation of cross-section under bending into account. For this purpose, Scarpa and Adhikari (2008) deprived equivalent parameters of beam considering shear effects and obtained the results on tensile modulus and bending modulus of SWCNTs, which were verified by previous literatures. Later Scarpa, Adhikari and Phani (2009) and Scarpa, Adhikari, Gil and Remillat (2010) respectively used the same method to study elastic mechanical properties of GS. Kuzkin and Asonov (2012) proposed a Timoshenko beam model based on longitudinal, shear, bending, and torsional stiffnesses for calibrate a vector-based model. Berinskii, Krivtsov, and Kudarova (2014) proposed a discrete mechanical model of monolayer graphene based on the energy of small strains on micro- and macroscales and estimated the bending stiffness of a graphene sheet corresponding to the Bernoulli-Euler model and the Timoshenko model respectively. Further Wang, Lan, Liu, Tan and He (2013) proposed a Timoshenko deep beam model with 3-node beam element to consider the flexibility of C-C bond and simulate the wrinkling of GS.

The aforementioned researches mainly focus on the flexibility of C-C bonds by correcting the beam cross-section attributes or altering potential functions. Very few efforts have been made on the flexibility in the joint of C-C bond, while it is a meaningful work. Because the joint of C-C bond is rigid in previous model, which will lead the rotation angle between adjacent C-C bonds in the position of rigid joint to be almost a constant value when bending mechanism occurs. Nevertheless, the relative rotation angle between adjacent C-C bonds will alter when any deformations occur in reality. Therefore the published models cannot well simulate this flexibility of joint. Shi, Yang, and Atluri (1987) presented a flexible-joint frames model which used a large bending flexibility short beam to link the girder in the joint for accomplishing the change of rotation angle between adjacent sticks.

This paper makes the most of this conceive and establishes a variable cross-Section 3-node Timoshenko beam to simulate C-C bond. The flexibilities of C-C bond and C-C bond joint are taken into account simultaneously. After that, we take an annular graphene sheet (AGS) as research object, which is popularly used in nanoelectronics by Schelter, Recher, and Trauzettel (2012), and made the study of wrinkling of AGS.

The paper is structured as follows. In Section 2, an improved MSM methodology is proposed based on classical MSM approach. Next, the stiffness matrix of variable cross-Section 3-node Timoshenko beam method is deduced for later calculation. In Section 3, wrinkling characteristics of AGS under circular shearing at inner edge are studied by iMSM method, and a predicted modal is used to evaluate our results. In Section 4, the parametric studies of beam parameters on AGS wrinkling are accomplished. Finally the paper ends up with some concluding remarks In Section 5.

2. Methodology details

For clarity of the paper, we make the further explanations for considering flexibility in the joint of C-C bond in detail. Usually beams simulation the C-C bonds are rigidly connected with each other, which means that this joint of C-C bond is rigid and can transfer bending moment and shear force when the structure is loaded. In this situation, the angle between the C-C bonds (rigid joint) keeps a constant or has a tiny change which can be neglected comparing with the deformation of the whole structure. However, the adjacent covalent bond will make a relative rotation in actual bending deforming process when the graphene structure is loaded by Odegard, Gates, Nicholson and Wise (2002) and Li and Chou (2003). It is obvious that the rotation angle exists and cannot be neglected in the joint of C-C bond.

This fact guides us to take the flexibility in the joint of C-C bond into account. Considering low efficiency of using rotating spring to represent the joint by Yan and Shi (2010), we present using a short beam with large bending flexibility near the joint to simulate the joint flexibility of C-C bond, as shown in Fig. 1. Actually this approach is an approximate method to achieve the rotation between the adjacent beams. Although the joint is still rigid in essence, the length of short beam with large bending flexibility is very small comparing with the length of whole beam, the rotation between the adjacent beams can be realized in some extent.