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Mechanical properties of double-layered graphene sheets

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ABSTRACT

In this paper, the molecular structural mechanics method is employed to calculate the mechanical properties of a double-layered carbon graphene sheet more accurately. For this purpose, covalent bonds are modeled using nonlinear beam elements and van der Waals interactions are replaced by nonlinear truss elements. Morse potential and Lennard–Jones potential equations are used to simulate the covalent bonds and van der Waals interactions, respectively. For each atom, van der Waals forces are considered with respect to all the other atoms located in its cut-off radius. In addition to in-plane mechanical properties of single and double-layered graphene sheets some out-of-plane properties like the thickness-wise stiffness and shear modulus are studied. The results indicate that Young's modulus of a double-layered carbon graphene sheet decreases linearly with strain while Poisson's ratio is independent from it. Also it is noted that the thickness-wise stiffness significantly increases while the distance between the two layers declines however the shear modulus is independent from shear strain.

1. Introduction

Due to their abundance in nature, graphene sheets can be economically used in various applications such as composite materials in order to increase their stiffness characteristics. Graphene Sheets (GSs) may exist as single-layered or multi-layered structures. It is possible to harness the multifunctional properties of graphene sheets to design innovative strain sensors and novel classes of advanced composites with superior mechanical and electric performance [1–4].

In modeling mechanical properties of nanostructures, theoretical studies have become more prevalent since experimental methods encounter many technological challenges [5]. Countless advances in Nanotechnology and its broad applications have motivated researchers to develop new methodologies for the analysis of physical properties of such new materials.

Using an assumed potential, Nicholson and Bacon [6] developed a simple lattice model with force constants. Kudin et al. [7] used Ab initio methods and predicted Young's modulus and Poisson's ratio of a GS to be 1.02 TPa and 0.149, respectively. However, Van Lier et al. [8] reported a 1.11 TPa value for Young's modulus of a graphene sheet using Ab initio method.

Equivalent atomistic continuum–structural mechanics approach, which uses typical structural mechanics elements such as rods, beams and shells, can also been utilized to simulate the static and dynamic behavior of nanostructures [9,10]. Due of its robustness and ease, several authors employed Molecular Mechanistic (MM) modeling approach to achieve single-layer graphene sheets' properties.

A finite element model based on modified Morse potential has been developed to simulate graphene and carbon nanotube structures' properties by Meo and Rossi [11]. Tserpes and Papanikos [12] also used a finite element model to identify the thickness and stiffness properties of an equivalent material associated to the carbon bonds represented by beams in Single-Walled Carbon Nanotubes (SWCNTs). Later on Sakhaee-Pour et al. [13] used Tserpes and Papanikos's [12] approach to compute natural frequencies and mode shapes of single-layered graphene sheets. Using the molecular structural mechanic, wave propagation characteristics, vibration behavior and the thickness and in-plane mechanical properties of single-layered graphene sheet are studied in [14–16].

The elastic behavior of multi-layered graphene sheet (MLGS) and multi-wall carbon nanotubes has been simulated by Chunyu and Li [17] using molecular mechanic method. In order to make the computation more convenient, they considered the van der Waals interactions between adjacent layers in a small cut-off radius and estimated Young's modulus to be 1.05 TPa for the MLGS. However, the experimentally-derived value of Young's modulus was 1.025 TPa [18,19]. Bao et al. [22] employed the Molecular Dynamics (MD) simulation and reported a negligible difference in Young's modulus for single-layered and multi-layered graphite. Scarpa and et al. [20] using the molecular structural mechanic demonstrate that the mechanical behavior of double layered graphene can be approximated by a first order shear deformation theory mutated from the analysis of structural sandwich beams and panels, in their approach the upper and lower graphene sheets

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are modeled using the Timoshenko Finite Element beams and also van der Waals interactions are simulated by using the nonlinear springs. Later on Chandra et al. [21] follow this approach to study the vibrational characteristics of double-layered graphene sheets.

A review of the literature reveals that in all MSM works conducted thus far to calculate the mechanical properties of the double-layered graphene sheets, both covalent bonds and van der Waals interactions have not been considered nonlinearly together and the out of plane properties of DLGS are not studied directly. Considering the nonlinear behavior of both covalent bonds and van der Waals interactions motivated this study to present a finite element solution to estimate the both in plane and out of plane mechanical properties of DLGS.

Therefore, in this paper a modified molecular structural mechanics method is adopted to assess the mechanical properties of MLGSs in the presence of interlayer van der Waals interactions. Van der Waals forces are applied on each atom from all adjacent atoms within its cut-off radius range. To this end, covalent bonds and van der Waals interactions are modeled using nonlinear beam and truss rod elements respectively. Young's, shear, and bending moduli, and Poisson's ratio of single- and double-layered graphene sheets are calculated. The thickness wise stiffness values are also estimated for two adjacent layers. The results obtained in the present work are compared with those reported in the literature.

2. Covalent bonds modeling

In the present atomistic simulation, equivalent structural beams are employed to simulate the covalent bonds during finite element solution. In order to model inter-atomic forces, the elastic properties of the beam are computed using covalent bonds stiffness coordinates.

By considering the equivalent potential energies of the molecular and structural mechanics, the properties of the beam have been developed [10]. For this purpose, force field constants of the covalent bonds are used as follows:

$$\frac{EA}{r_0} = k_r, \frac{EI}{r_0} = k_\theta, \frac{GJ}{r_0} = k_\phi \tag{1}$$

where E denotes modulus of elasticity and G stands for shear modulus of the beam. Force field constants k_r, k_θ, and k_ϕ represent bond stretching, angle bending and torsional stiffness of the covalent bonds, respectively. A is the cross sectional area, I is the area moment of inertia, J is the polar moment of inertia, and r_0 denotes the length of the beam. The length is assumed to be equal to the covalent bond distance of the carbon atoms in the hexagonal lattice. Assuming a circular cross section for the beam, Eq. (1) results in [17]:

$$d = 4\sqrt{\frac{k_\theta}{k_r}},\ E = \frac{k_r^2 r_0}{4\pi k_\theta},\ G = \frac{k_r^2 k_\phi r_0}{8\pi k_\theta^2} \tag{2}$$

where d is the cross section diameter of the beam. Inter-atomic forces of the bonded carbon atoms were also modeled through the equivalent structural beams. The force constants k_θ and k_ϕ are considered 8.76×10^{-10} N nm/Rad^2 and 2.78×10^{-10} N nm/Rad^2 respectively. However, k_r is obtained from the second derivative of the Morse potential equation, i.e. Eq. (3):

$$k_r = E'' = 4\beta^2 D_e e^{-2\beta(r-r_0)} - 2\beta^2 D_e e^{-\beta(r-r_0)} \tag{3}$$

where r_0 is the bond equilibrium length, D_e is the dissociation energy and β is a curve fitting parameter. So a covalent bond can be replaced by a 6 DOF nonlinear beam characterized by Eqs. (2) and (3).

3. Van der Waals interaction modeling

Layers of a multi-layered graphene sheet are stacked together through van der Waals forces. The van der Waals force is a non-bonded interaction, and it can be an attraction or a repulsion force. Attraction occurs when a pair of atoms approach each other within a certain distance, and repulsion occurs when the distance between the interacting atoms becomes less than 3.81637 Å. These interactions are often modeled with the Lennard–Jones potential function [23]. Some researcher consider only infinitesimal deformation of a CNT or graphene Thus, the van der Waals forces are estimated by the Taylor expansion to the first-order around the equilibrium position prior [24,25] Some other researcher uses nonlinear finite element considering the nonlinear spring element in their model each atom of the bond laying in one layer is connected to the nearest and near neighbor in the opposite plane [20,21]. In the present model the similar approach with the nonlinear spring is used. The stiffness between a pair of atoms (k) can be obtained from the second derivation of the Lennard–Jones potential:

$$k(r) = 24\frac{\varepsilon}{\sigma^2}\left[26\left(\frac{\sigma}{r}\right)^{14} - \left(7\frac{\sigma}{r}\right)^{8}\right] \tag{4}$$

where r is the distance between interacting atoms, and ε and σ are the Lennard–Jones parameters. It is clear that the van der Waals force between two atoms is highly nonlinear. Therefore, the truss rod connecting the atoms is a three-DOF nonlinear element with its stiffness relationship obtained from Eq. (4).

4. Results and discussion

To simulate the non-linearity of beams and truss rods, a displacement-based finite element solution is adopted. To this end, a computer code is written in FORTRAN which is able to assemble a 12-DOFs beam element stiffness matrix with a 6-DOFs truss rod element stiffness matrix. The prescribed displacement is divided into a number of increments. After applying the displacement increments at each step, the stiffness matrix and the geometry of the graphene sheet are updated and then the solution continues for a new increment.

In this section results for both Zigzag and Armchair, single and double layer GSs (as indicated in Fig. 1) from the presented finite element model are reported and discussed. These results include Young's, shear and bending moduli and Poisson's ratio of single and double-layered graphene sheets. The cross section of the FEM model of the double-layered graphene sheet is shown in Fig. 2. It should be noted that in the present study, all the predictive equations are constructed using the curve fitting method and the accuracy of this method is measured using a multiple coefficient of determination, R^2, in which this value has been found to be greater than 0.98 for all cases.

4.1. In plane stiffness

Young's modulus is defined as the first derivation of stress versus strain i.e.:

$$E = \frac{d\sigma}{d\varepsilon} \tag{5}$$

where $\sigma = F/A$, F is the total reaction force, $A = b \times t$ is the cross-sectional area, b is the MLGS width and t is the SLGS thickness which is taken 0.34 nm [10]. The stress–strain curve of the graphene sheet is illustrated in Fig. 3. From this figure it is observed that the curves of Zigzag and Armchair graphene are similar in both single- and double-layered sheets. However, the slope of this curve decreases with increasing strain.