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Comparative study on predicting Young's modulus of graphene sheets using nano-scale continuum mechanics approach

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ABSTRACT

In this research, nano-scale continuum modeling is employed to predict Young's modulus of graphene sheet. The lattice nano-structure of a graphene sheet is replaced with a discrete space-frame structure simulating carbon-carbon bonds with either beam or spring elements. A comparative study is carried out to check the influence of employed elements on estimated Young's moduli of graphene sheets in both horizontal and vertical directions. A detailed analysis is also conducted to investigate the influence of graphene sheet sizes on its Young's modulus and corresponding aspect ratios that unwelcomed end effects disappear on the results are extracted. At the final stage, defected graphene sheets suffering from vacancy defects are investigated through a stochastic analysis taking into account both number of defects and their locations as random parameters. The reduction level in the Young's moduli of defected graphene sheets compared with non-defected ones is analyzed and reported.

1. Introduction

A new generation of polymeric composites has blossomed over the last decades owning to the discovery of nano-materials as a new generation of reinforcing agents. Among them, a considerable attention have been devoted to carbon nanotubes (CNT) and graphene sheets due to their extraordinary and unique properties from different mechanical, electrical and thermal aspects. Although CNTs and graphene sheets present almost the same class of mechanical properties, graphene is preferred to CNT when certain thermal and electrical properties are focused [1].

A fundamental step prior to understanding mechanical behavior of graphene reinforced polymers is characterizing mechanical properties of isolated graphene. Tremendous limitations exposed to the context of nano-scale experimental measurements have stimulated researchers to pursue different theoretical modeling techniques. Generally, modeling techniques at nanoscale are classified into three main categories of atomistic modeling, continuum modeling and nano-scale continuum modeling [2]. Atomistic modeling methods are suffering from intensive computational efforts and complicated formulations. Moreover, they cannot be applied to the systems with large numbers of atoms. Continuum models are constructed on the basis of Elasticity theories by replacing a lattice structure of CNT/graphene with a simple continuum medium. The validity of continuum modelings are required to be studied carefully where a real discrete structure of CNT/graphene is neglected. Nano-scale continuum models are identified as those modeling techniques where continuum assumptions are applied to the molecular bonds instead of the whole nano-structure [2]. In these techniques, each C-C bond is replaced with a continuum element while the discrete nature of the nano-structure is not violated. The replacement of C-C bonds with equivalent elements appearing in the variety forms of beam, rod, truss or spring is accomplished by establishing a linkage between molecular configurations and solid mechanics. Different researchers have used nano-scale continuum mechanics to analyze the mechanical behavior of CNTs using either linear or nonlinear elements [3–17]. The majority of nano-scale modeling techniques have been carried out numerically, while very rare studies have been performed analytically [4–6,13].

Limited studies have been concentrated specifically on graphene sheets in literature. Meo and Rossi have modeled graphene sheets employing translation and torsional spring element for simulating bond stretching and bond angle variations. They have employed nonlinear interatmoic potentials in their study [9]. Shokrieh and Rafiee [13] have developed a closed form solution for predicting Young's moduli of a graphene sheet in two orthogonal directions substituting the lattice structure of a graphene sheet with a honeycomb-like discrete structure. In some studies, the Young's modulus of a graphene sheet is evaluated employing atomistic modeling techniques [18,19]. Some other investigators have originally predicted the Young's modulus of CNTs versus CNT radius and then estimated the Young's modulus of a

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graphene sheet relying on this fact that a graphene sheet can be virtually viewed as a CNT with infinite radius [4,6]. Zhang et el. [20] have predicted the mechanical properties of a bilayer graphene sheet coupled by sp^3 bonding using molecular dynamics (MD) simulation. Investigating the influence of Stone-Wales defects on the tensile properties of a graphene sheet, Ren an Cao [21] have reported that this type of defect does not have any influence on the Young's modulus and Poisson's ratio using density functional theory. Elastic mechanical properties of graphene sheets have been computed by Georgantzinos and his co-workers using spring elements and incorporating either linear or nonlinear interatomic potential [22,23]. Recently, Javvaji et al. [24] have extensively investigated the effect of domain size, lattice orientation and crack length on the mechanical properties of graphene employing MD simulations.

The main objective of this article is to perform a comparative study on different nano-scale continuum mechanics approaches for extracting Young's modulus of graphene nanostructure. The influence of linear and non-linear models on the results will be also investigated. Moreover, both defected and non-defected graphene sheets are simulated and analyzed to investigate the degree to which structural defect will influence the Young's modulus on the basis of employed modeling technique.

2. Morphology of graphene sheets

Graphene layers is considered as the building units of Graphite which are stacked together with interlayer spacing of 0.34 nm [2]. Graphene can be imagined as a single layer of covalently bonded carbon atoms arranged in the periodic hexagon rings resembling honeycomb lattice configuration (See Fig. 1). The length of carbon-carbon (C-C) bond in graphene layer is nearly 0.142 nm.

3. Molecular interactions

In the context of molecular studies, total inter-atomic potential energy of a molecular system is regulated by the contribution of individual bonding and nonbonding interactions as below [25]:

$$E_{tot} = U_r + U_\theta + U_\varphi + U_\omega + U_{VdW} + U_{es} \tag{1}$$

where U_r, U_θ, U_φ, and U_ω are representative of bond stretching, bond angle variation, dihedral angle torsion and out-of-plane torsion, respectively. U_{VdW} and U_{es} are associated with non-bonded van der Waals (vdW) and electrostatic interactions. Non-bonded interactions are negligible in comparison with bonded ones. The merged form of dihedral angle torsion and out-of-plane angle torsion is expressed as below [25]:

$$U_\tau = U_\varphi + U_\omega \tag{2}$$

Thus, total inter-atomic potential energy of a nano-structure is reduced to contain bond stretching (U_r), bond angle variation (U_θ) and torsional (U_τ) terms. Among bonded interactions, the dominant parts of inter-atomic potential are bond stretching and bond angle variations due to their significant contribution in comparison with other interactions especially when the graphene is subjected to small in-plane deflections.

Linear representation of total interatomic potential energy of a molecular system can be approximated using harmonic functions as below:

$$E_{tot}^L \cong U_\rho + U_\theta + U_\tau = \frac{1}{2}k_r(\Delta r)^2 + \frac{1}{2}k_\theta(\Delta\theta)^2 + \frac{1}{2}k_\phi(\Delta\varphi)^2 \tag{3}$$

where, reflected force constant in above equation are introduced as below using AMBER force field [26]:

$$k_r = 938\left[\frac{\text{kcal}}{\text{mole}} \times \frac{1}{\text{nm}^2}\right] = 6.52 \times 10^{-7}\left[\frac{\text{N}}{\text{nm}}\right] k_\theta = 126\left[\frac{\text{kcal}}{\text{mole}} \times \frac{1}{\text{rad}^2}\right]$$
$$= 8.76 \times 10^{-10}\left[\frac{\text{N nm}}{\text{rad}^2}\right] k_\varphi = 40\left[\frac{\text{kcal}}{\text{mole}} \times \frac{1}{\text{rad}^2}\right] = 2.78 \times 10^{-10}\left[\frac{\text{N nm}}{\text{rad}^2}\right] \tag{4}$$

Non-linear representation of total interatomic potential energy is estimated using modified Morse potentials as below [27]:

$$E_{tot}^{NL} \cong U_\rho + U_\theta = D_e\{[1 - e^{-\beta(r-r_0)}]^2 - 1\} + \frac{1}{2}k_\theta(\theta - \theta_0)^2[1 + k_{sextic}(\theta - \theta_0)^4] \tag{5}$$

where:

$$D_e = 6.03105e^{-19}\,[\text{N m}],\ \beta = 2.625e^{10}\,[\text{m}^{-1}],\ r_0 = 0.142\,[\text{nm}]. \tag{6}$$

$$k_\theta = 0.9e^{-18}\left[\text{N}\frac{\text{m}}{\text{rad}^2}\right],\ k_{sextic} = 0.754\,[\text{rad}^{-4}],\ \theta_0 = 2.094\,[\text{rad}] \tag{7}$$

In the next section, E_{tot}^L and E_{tot}^{NL} are used separately to construct linear and non-linear Finite Element (FE) models of a graphene sheet, respectively.

4. Finite element modeling

In the field of nano-scale continuum modelings, there are two broadly used strategies in modeling CNT or graphene nano-structure recognized as beam-based or spring-based models. Following the fundaments of nano-scale continuum modeling techniques, the later uses spring elements to capture mechanical behavior of C-C bonds while the former exploits beam elements for constructing FE model. The fundaments of these modeling techniques are outlined in this section which will be used for the purpose of comparative study. It is worth mentioning that in both categories, linear and non-linear elements can be used.

A computer code is written in APDL of ANSYS to construct geometrical model of a graphene sheet. In this model, structural nodes are placed at the exact location of carbon atoms in graphene sheet.

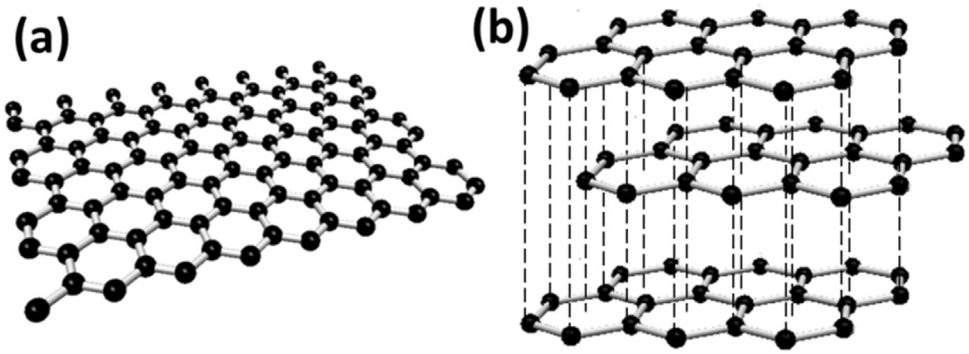

Fig. 1. (a) Lattice nano-structure of a graphene sheet, (b) Graphite consisting of stacked graphene sheets.