Structures 13 (2018) 131–138

Contents lists available at ScienceDirect

Structures

journal homepage: www.elsevier.com/locate/structures

Effects of Size and Shape on Elastic Constants of Graphene Sheet

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ARTICLE INFO

Keywords:
Nanostructures
Mechanical properties
Strength
Finite element analysis (FEA)

ABSTRACT

Nanotechnology is used in different engineering fields such as mechanical, aerospace, and civil. One of the most interesting structures which recently have come to the center of attention is the Graphene Sheet (GS). Graphene is a material with high potential of usage in civil structures like structural rehabilitation. In the present paper a finite element based structural analysis program is employed to study the mechanical properties of GS. The advantage of using this method is its simplicity and efficiency in different types of loading. The models considered here are based on a structural mechanics approach by using finite beam elements. Variations of Young's moduli of GS versus different sizes of sheet in two principal directions are investigated. Afterwards, Poisson's ratio and shear modulus for a special case are obtained. The results are consistent with basic structural mechanics theory. Final results reveal the importance of GS size on its Young's modulus, Poisson's ratio and shear modulus. The results are in good agreement with previously published results by other scientists.

1. Introduction

Exciting properties of nanostructures such as Carbon Nanotube (CNT) led to discovery of a new nanostructure, namely the Graphene Sheet (GS). GS is a mono layer of carbon atoms arranged in a hexagonal lattice and is widely used to characterize carbon based materials including graphite. This 2D nanomaterial is the thinnest known material in the world and the strongest ever encountered [1]. Recently new methods have been developed to mass produce GS in an economical manner [2,3].

The prospects of this new material have motivated numerous researches to find potential applications. Small size, excellent physical properties, high stiffness, low density and excellent electronic and thermal properties [4–9] are some of the exciting properties of GS with an abundant spectrum of application in fields such as chemistry, physics, mechanics, material science and engineering. It should be noted that its strong two dimensional layer structure makes GS potential reinforcement in nanocomposites [10,11]. Use of GS as reinforcement in composites is a beginning for world bursting with Graphene application. This class of new material by some of its great property, like potential application in radar absorbing system and batteries will gain more attention by the progress in this field [12]. Owing to the importance of the mechanical properties of GS, researchers worldwide have tried different approaches including experimental, elastic continuum and molecular dynamics (MD) to obtain its mechanical properties [13–15]. Because of the difficulties of experimental work on GS, many researchers have resorted to computational approaches to investigate its behavior [16]. These approaches include atomistic and continuum modeling methods. Atomistic modeling such as Quantum mechanics (QM) and molecular dynamics (MD) simulations are often used to study the defects on mechanical properties of GSs and CNTs. Although atomistic modeling approaches provide accurate results, they are extremely complicated and time-consuming.

Approaches based on Continuum mechanics use well-known structural elements such as beams, shells and plates to simulate GS structures. These approaches are simple and provide acceptable results in smaller computational time durations. Hybrid approaches such as atomistic based finite element modeling have also been used to analyze GS and other carbon based nanostructures in many recent works due to its computational cost and CPU time advantages [17].

Previous studies on Graphene were devoted to obtain the mechanical properties such as Young's modulus, Poisson's ratio or shear modulus. In 2003 Li and Chou [14] used a structural mechanics approach to determine Young's modulus and shear modulus of carbon nanotubes and GS. They evaluated the Young's modulus as 1.033 TPa which was slightly dependent to its size. In 2010 Shokrieh and Rafiee [15], by using nanoscale continuum mechanics approach, predicted that the Young's modulus of GS would be about 1.04 TPa. Arroyo and Belytschko [18] calculated the Poisson's ratio as equal to 0.412. They used Brenner's potential which had been previously used by Kudin et al. [19].

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https://doi.org/10.1016/j.istruc.2017.12.005
Received 27 January 2017; Received in revised form 22 October 2017; Accepted 13 December 2017
Available online 16 December 2017
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1.1. Research significance

In most of the accomplished works on nanostructures, extremely long and time-consuming computational methods have been employed. This issue raised vast efforts to present methodologies with more applicability and interest for practical engineering applications. In this study, a simple methodology is introduced which employs common structural analysis software based on the finite element method. The Young's modulus of GS in two principal directions is calculated. The Poisson's ratio of GS is also considered to confirm the method. The influence of the size including changing in length, width and area of the Graphene sheet on both Young's moduli and Poisson's ratios are investigated comprehensively. In comparison with previous works, the methodology is simpler and more efficient to be used for complicated large systems. Therefore it can be used in comprehensive parametric studies to assess the effects of various parameters.

2. Theoretical points

From the molecular mechanical approach, nanostructures such as GS can be considered as a large molecule made from carbon atoms. In this case, the atomic nuclei can be regarded as material points [14]. Arrangement and motion of atoms could be explained by the force field that is created by nucleus-nucleus and electron-nucleus interactions [20]. Usually the force field is expressed by steric potential energy that depends merely on the nuclei's relative coordinates. The general expression for total steric potential energy, ignoring the electrostatic interaction, could be obtained by energy summation due to bonded and non-bonded interactions as [21]:

$$U = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega + \sum U_{vdw} \tag{1}$$

where U_r denotes the bond stretch potential, U_θ is the bond angle bending potential, U_ϕ is the potential pertaining to dihedral angle torsion, and U_ω represents the potential of the out of plane torsion. Moreover, U_{vdw} is van der Waals non-bonded interaction potential energy. Interatomic interactions are shown in Fig. 1.

A GS consists of carbon atoms that are arranged in a monolayer hexagonal lattice. Therefore the van der Waals potential energy, U_{vdw}, which exists between the layers can be ignored. Simple forms of potential energies can be expressed as follows [14,22]

$$U_r = \frac{1}{2}K_r(r - r_0)^2 = \frac{1}{2}K_r\Delta r^2 \tag{2}$$

$$U_\theta = \frac{1}{2}K_\theta(\theta - \theta_0)^2 = \frac{1}{2}K_\theta\Delta\theta^2 \tag{3}$$

$$U_\tau = U_\phi + U_\omega = \frac{1}{2}K_\tau\Delta\phi^2 \tag{4}$$

where r and θ are distance between atoms and the bond angle after deformation, respectively. r_0 and θ_0 are the initial values in each case. Δr, $\Delta\theta$ and $\Delta\phi$ are bond stretching variation, bond angle variation and bond twisting variation, respectively [23]. K_r, K_θ and K_τ are bond stretch force constant, bond angle bending force constant and torsional resistance constant, respectively. In Eq. (4), U_ϕ is the total potential energy due to out of plane torsion and dihedral angle torsion.

According to the paper by Li and Chou [14], similarities are found between these energies and energies used in structural mechanics for beams. As shown in Fig. 2, potential energy of a homogenous beam with length of L and cross section of A, due to axial deformation, ΔL, can be expressed as [15]:

$$U_A = \frac{EA}{2L}(\Delta L)^2 \tag{5}$$

where E is the elastic modulus of beam material. Potential energy due to bending can be obtained as

$$U_M = \frac{EI}{2L}(2\alpha)^2 \tag{6}$$

where α and I represent the rotation angle and second moment of area of cross section of the beam, respectively. Torsional potential energy can be obtained in a similar manner as:

$$U_T = \frac{GJ}{2L}(\Delta\beta)^2 \tag{7}$$

where $\Delta\beta$, G and J are the twist angle at two ends of the beam, shear modulus and polar second moment of area for beam's cross section, respectively. Similarities between intermolecular potential energies and structural potential energies of beam yield

$$K_r = \frac{EA}{L} \tag{8}$$

$$K_\theta = \frac{EI}{L} \tag{9}$$

$$K_\phi = \frac{GJ}{L} \tag{10}$$

The values of K_r, K_θ and K_ϕ can be obtained from different sources [24] as

$$K_r = 652\,\text{nN/nm} \tag{11}$$

$$K_\theta = 0.876\,\text{nN}\cdot\text{nm}/rad^2 \tag{12}$$

$$K_\phi = 0.278\,\text{nN}\cdot\text{nm}/rad^2 \tag{13}$$

These values can be used to evaluate structural characteristics of the beam used in the simulation. Values of d (diameter of a bond), E and G can be obtained for a carbon-carbon bond by using Eqs. (8)–(10) as

$$d = 4\sqrt{\frac{K_\theta}{K_r}}, \quad E = \frac{K_r{}^2L}{4\pi K_\theta}, \quad G = \frac{K_r{}^2LK_\phi}{8\pi K_\theta{}^2} \tag{14}$$

Substituting for the amount of L (the bond length) as 0.142nm in a hexagonal lattice, the other parameters can be obtained. Engineering properties used in model are given in Table 1.

3. Simulation

From the civil engineering viewpoint, at first sight we could consider GS as a truss (at first sight, using engineering judgement), but not a real truss. Its feature reminds a truss and that is the reason of our study to expand our field far away. In fact because of its bending moment, GS should be considered as a frame in which the carbon-carbon bond acts like a finite beam member. In order to have the frame behave like a GS, the members of frame are modeled by beam elements whose axial stiffness can be obtained from Eq. (8). Also, the connections between the members of the frame are modeled in accordance with the rotational stiffness values in Eqs. (9) and (10). Hence, the frame model of a GS would experience similar deformations to those of the GS due to in plane arbitrary external forces. In order to model the bond angle variation, a rotational spring (as shown in Fig. 3) with stiffness of k_θ is used.

In order to model the torsional and dihedral deformations between the bond elements, a rotational spring with total stiffness of k_ϕ is used to consider the influences of the mentioned interactions between elements.

For axial deformation, a spring with stiffness of k_r is used as shown in Fig. 4. Using knowledge of elasticity, by having constants such as E, I, A, G and L, the axial behavior of a rod can be modeled with a spring like Fig. 4.

In this study, a bar is used for axial behavior of a bond and two springs are used for dihedral and bending behavior of the GS. In order to visualize the degrees of freedom, a single hexagonal GS has been shown in Fig. 5.

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