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An atomistic-based continuum approach for calculation of elastic properties of single-layered graphene sheet

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ABSTRACT

The elastic deformation of a single-layer nanostructured graphene sheet is investigated using an atomistic-based continuum approach. This is achieved by equating the stored energy in a representative unit cell for a graphene sheet at atomistic scale to the strain energy of an equivalent continuum medium under prescribed boundary conditions. Proper displacement-controlled (essential) boundary conditions which generate a uniform strain field in the unit cell model are applied to calculate directly one elastic modulus at a time. Three atomistic finite element models are adopted with an assumption that the force interaction among carbon atoms can be modeled by either spring-like or beam elements. Thus, elastic moduli for graphene structure are determined based on the proposed modeling approach. Then, effective Young's modulus and Poisson's ratio are extracted from the set of calculated elastic moduli.

Results of Young's modulus obtained by employing the different atomistic models show a good agreement with the published theoretical and numerical predictions. However, Poisson's ratio exhibits sensitivity to the considered atomistic model. This observation is supported by a significant variation in estimates as can be found in the literature. Furthermore, isotropic behavior of in-plane graphene sheets was validated based on current modeling.

1. Introduction

Recently, nanostructured graphene sheets have captured the attention of many researchers. This can be attributed to their remarkable mechanical properties and cheap method of production as presented by Stankovich et al. [1]. In addition, characterization of behavior of graphene facilities better understanding of other fundamental nano-materials like Carbon nanotubes (CNTs) which are viewed as a deformed graphite sheets.

The complexity and high expense of investigating the mechanical behavior of graphene sheets via experiments stimulated the use of numerical simulation as proven tool capable of modeling nanostructures with different dimensions. In this context, equivalent continuum-structural mechanics has been widely used to characterize the mechanical behavior of nanostructured materials. In this approach, typical elements of structural mechanics such as rods, beams and shells are used to simulate the static and dynamic behavior of monolayer graphene. The mechanical properties of such structural elements are derived from the equivalence between steric potential of the carbon–carbon (C–C) bonds and mechanical strain energies associated with tension, torsion and bending related to the mechanical elements simulating the bonds themselves. A truss model was proposed by Odegard et al. [2], wherein rods of different degrees of stiffness represent the stretching and in-plane bending capabilities of the C–C bonds. Li and Chou [3] proposed an equivalent structural beam capable of modeling interatomic forces of the carbon covalent bonds. They adopted a molecular structural mechanics approach to compute effective elastic constants of carbon nanotubes. Meo and Rossi [4] developed a finite element model based on the use of nonlinear central spring and linear torsional spring elements to represent the modified Morse potential when simulating graphene. Cho et al. [5] carried out a molecular structural analysis to predict the elastic constants of graphite. The in-plane properties of graphite were derived by considering a single-layer graphene sheet subjected to an in-plane loading. Based on atomistic finite element approach, Shakhaee-Pour [6] investigated the elastic behavior of single-layer graphene sheets. By employing an equivalent structural beam, the elastic constants of graphene were calculated. Scrape et al. [7] proposed a truss-type model in conjunction with cellular material mechanics theory to describe the in-plane elastic properties of single-layer graphene sheets.

Analytically, some researchers [8] investigated Young's modulus of graphene and CNTs based on nanoscale continuum modeling. They employed frame elements to simulate C–C bonds for which they obtained a closed form solution. Several others utilized atomistic finite elements to simulate graphene sheet using linear interatomic potential functions for bonds. Atomistic-based finite element models have been used to analyze graphene sheets in many

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recent studies in literature due to its simplicity, computational cost effectiveness and low CPU time. In contrast, atomistic models require a significant computational effort. Taking into account the advantages of the atomistic models, FE incorporates actual atomistic characteristics and interatomic forces among carbon atoms while other continuum models fails to do so. Georgantzinos et al. [9] developed a formulation on the basis of spring element using linear interatomic potentials to compute mechanical properties. Some other researchers incorporated non-linear springs for simulating both bond stretch and bond angle variation [10,11]. Based on an equivalent continuum approach, Alzebdeh [12] used atomistic finite element simulation in conjunction with a beam model to evaluate elastic moduli and constants for single-layered graphene sheets with different sizes.

In this paper, a continuum approach based on an atomistic modeling is proposed to simulate mechanical behavior of graphene, in order to predict its mechanical properties. At nanoscale, we consider a unit cell representing a finite-size graphene sheet equivalent to a homogenized medium in a continuum sense. Three atomistic finite element-based models for bond stretch and bond angle variation are adopted: (i) linear spring, (ii) nonlinear spring, and (iii) structural beam to model interatomic interactions between carbon atoms, described by modified Morse potential function.

2. Molecular interactions

From the viewpoint of molecular mechanics, the nanostructure of a graphene sheet is constituted by a monolayer of carbon atoms arranged periodically and uniformly in a hexagonal "honeycomb" fashion (as shown in Fig. 1).

Their motion is governed by the molecular force field, which is generated from electron–nucleus and nucleus–nucleus interactions. The total interatomic potential energy of a molecular system is expressed as a sum of several energy terms after neglecting the non-bonded interactions:

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

where U_r stands for a bond stretch, U_θ is for a bond angle bending, $\sum U_\varphi$ is for dihedral angle torsion, and U_ω is for an improper (out-of-plane) torsion. Several different potential functions for describing the carbon–carbon bond other than simple harmonic functions are available [13,14]. The Tersoff–Brenner potential function is generally more accurate compared to other potential functions but it is complicated as presented by Jiang et al. [15]. Considering a single-layered sheet, generally, the dominant parts of interatomic potential are bond stretching and bond angle variations due to their significant contribution comparing to other interactions. The modified Mores potential function in Belytschko et al. [16] is simple and therefore, will be adopted in the present study as given below:

$$U = U_{strech} + U_{angle} \tag{2}$$

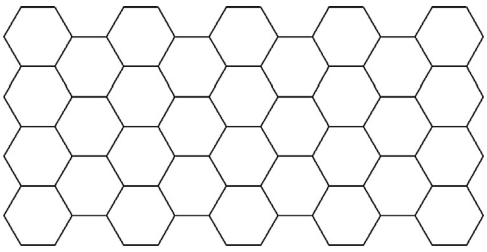

Fig. 1. Geometry of a graphene sheet.

$$U = D_e\{[1 - e^{-\beta(\Delta r)}]^{-2} - 1\} \tag{3}$$

$$U = \frac{1}{2}k_\theta(\Delta\theta)^2[1 + k_{sextic}(\Delta\theta)^4] \tag{4}$$

where U_{strech} is the bond energy due to bond stretch, and U_{angle} is the bond energy due bond angle variation. The above parameters (constants) are calibrated by Belytsckho [16] with Brenner potential as follows:

$$D_e = 0.6031 \text{ nN nm}, \quad \beta = 26.25 \text{ nm}^{-1}$$

$$k_\theta = 8.7e-10 \text{ nN} \cdot \frac{\text{nm}}{\text{rad}^2}, \quad k_{sextic} = 0.755 \text{ rad}^{-4}$$

This set of parameters corresponds with the Brenner potential for strain below 10% and separation (dissociation) energy of 124 kcal mol [17]. The modified Morse interatomic potential energies and force fields will serve as a basis for the current atomistic modeling and subsequent calculations.

3. Modeling technique

The proposed atomistic-based continuum approach for modeling of graphene sheets is presented. The basic idea is to use a representative unit cell at atomistic scale for repeating honeycomb geometry of graphene sheet with finite dimensions (Fig. 2). To calculate effective elastic moduli, an equivalent homogenized medium of a triangular shape with equal mechanical properties is assumed. This equivalence is established by equating energies of both models under controlled boundary conditions which generates a uniform (constant) strain field over the domain of unit cell. Potential energy stored in the atomistic model is determined via atomistic finite element simulations as will be outlined later.

3.1. Equivalent continuum model

For a homogeneous continuum medium, the constitutive relationship under a plane stress assumption is expressed in terms of the stiffness matrix C_{ij} by:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \end{Bmatrix} \tag{5}$$

Each entry (C_{11}, C_{22}, C_{12}) of the stiffness matrix is calculated by conducting a simulation run under prescribed loading conditions on boundaries. C_{66} is not an independent modulus; therefore its calculation will not be considered. Equivalently, the simulation models are run by applying a uniform strain (ε_{ij}^o) to the continuum model generating prescribed displacements on the boundaries given by:

$$u_i = \varepsilon_{ij}^o x_j \quad i,j = 1,2 \tag{6}$$

where u_i is the prescribed displacement, and x_j is the coordinate of boundaries. The corresponding continuum stored strain energy density is given by

$$U = \frac{V}{2}\sigma_{ij}\varepsilon_{ij} = \frac{V}{2}[C_{11}(\varepsilon_{11})^2 + C_{22}(\varepsilon_{22})^2 + C_{66}(\varepsilon_{12})^2 + C_{12}(\varepsilon_{11})(\varepsilon_{22})] \tag{7}$$

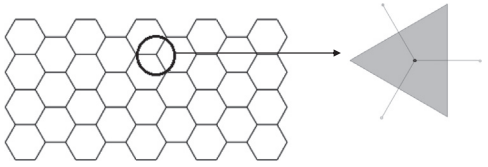

Fig. 2. Representative unit cell concept.